CalculiX CrunchiX USER'S MANUAL version 2.8p2

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1 Introduction.

This is a description of CalculiX CrunchiX. If you have any problems using the program, this document should solve them. If not, send us an E-mail (dhondt@t-online.de). The next sections contain some useful information on how to use CalculiX in parallel, hints about units and golden rules you should always keep in mind before starting an analysis. Section five contains a simple example problems to wet your appetite. Section six is a theoretical section giving some background on the analysis types, elements, materials etc. Then, an overview is given of all the available keywords in alphabetical order, followed by detailed instructions on the format of the input deck. If CalculiX does not run because your input deck has problems, this is the section to look at. Then, there is a section on the user subroutines and a short overview of the program structure. The last section contains a description of the verification examples you should have obtained along with the code of the program. If you try to solve a new kind of problem you haven't dealt with in the past, check this section for examples. You can also use this section to check whether you installed CalculiX correctly (if you do so with the compare script and if you experience problems with some of the examples, please check the comments at the start of the corresponding input deck). Finally, the User's Manual ends with some references used while writing the code.

This manual is not a textbook on finite elements. Indeed, a working knowledge of the Finite Element Method is assumed. For people not familiar with the Finite Element Method, I recommend the book by Zienkiewicz and Taylor [78] for engineering oriented students and the publications by Hughes [32] and Dhondt [18] for mathematically minded readers.

2 How to perform CalculiX calculations in parallel

Nowadays most computers have one socket with several cores, allowing for the calculations to be performed in a parallel way. In CalculiX one can

- solve the system of equations with the multithreaded version of SPOOLES. To this end
  - the MT-version of SPOOLES must have been compiled. For further information on this topic please consult the SPOOLES documentation

  - CalculiX CrunchiX must have been compiled with the USE_MT flag activated in the Makefile, please consult the README.INSTALL file.
  - at execution time the environment variable OMP_NUM_THREADS must have been set to the number of cores you want to use. In Linux this can be done by "export OMP_NUM_THREADS=n" on the command line, where n is the number of cores. Default is 1. Alternatively, you can set the number of cores using the environment variable CCX_NPROC_EQUATION_SOLVER. If both are set, the latter takes precedence.

- solve the system of equations with the multithreaded version of PARDISO. PARDISO is proprietary. Look at the PARDISO documentation how to link the multithreaded version. At execution time the environment variable OMP_NUM_THREADS must be set to the number of cores, default is 1.

- create material tangent matrices and calculate the stresses at the integration points in parallel. No special compilation flag is needed. At execution time the environment variable OMP_NUM_THREADS or the environment variable CCX_NPROC_RESULTS must be set to the number of cores, default is 1. If both are set, CCX_NPROC_RESULTS takes precedence. The maximum number of cores is detected automatically by CalculiX by using the sysconf(_SC_NPROCESSORS_CONF) function. It can be overriden by the user by means of environment variable NUMBER_OF_CPUS. Notice that if a material user subroutine (Sections 8.5 and 8.6) is used, certain rules have to be complied with in order to allow parallelization. These include (this list is possibly not exhaustive):
  - no save statements
  - no data statements
  - avoid logical variables
  - no write statements

- calculate the viewfactors for thermal radiation computations in parallel. No special compilation flag is needed. At execution time the environment variable OMP_NUM_THREADS or the environment variable CCX_NPROC_VIEWFACTOR must be set to the number of cores, default is 1. If both are set, CCX_NPROC_VIEWFACTOR takes precedence. The maximum number of cores is detected automatically by CalculiX by using the sysconf(_SC_NPROCESSORS_CONF) function. It can be overriden by the user by means of environment variable NUMBER_OF_CPUS.

- perform several operations in CFD calculations (computational fluid dynamics) in parallel. No special compilation flag is needed. At execution time the environment variable OMP_NUM_THREADS or the environment variable CCX_NPROC_CFD must be set to the number of cores, default

is 1. If both are set, CCX_NPROC_CFD takes precedence. The maximum number of cores is detected automatically by CalculiX by using the sysconf(_SC_NPROCESSORS_CONF) function. It can be overriden by the user by means of environment variable NUMBER_OF_CPUS.

- Calculate the magnetic intensity by use of the Biot-Savart law in parallel. No special compilation flag is needed. At execution time the environment variable OMP_NUM_THREADS or the environment variable CCX_NPROC_BIOTSAVART must be set to the number of cores, default is 1. If both are set, CCX_NPROC_BIOTSAVART takes precedence. The maximum number of cores is detected automatically by CalculiX by using the sysconf(_SC_NPROCESSORS_CONF) function. It can be overriden by the user by means of environment variable NUMBER_OF_CPUS.

- Perform several vector and matrix operations needed by the SLATEC iterative solvers or by ARPACK in parallel. To this end the user must have defined the environment variable OMP_NUM_THREADS, and used the openmp FORTRAN flag in the Makefile. The parallellization is done in FORTRAN routines using openmp. The corresponding lines start with "c$omp". If the openmp flag is not used, these lines are interpreted by the compiler as comment lines and no parallellization takes place. Notice that this parallellization only pays off for rather big systems, let's say 300,000 degrees of freedom for CFD-calculations or 1,000,000 degrees of freedom for mechanical frequency calculations.

Examples:

- For some reason the function sysconf does not work on your computer system and leads to a segmentation fault. You can prevent using the function by defining the maximum number of cores explicitly using the NUMBER_OF_CPUS environment variable

- You want to perform a thermomechanical calculation, but you are using a user defined material subroutine (Sections 8.5 and 8.6) which is not suitable for parallelization. You can make maximum use of parallelization (e.g. for the calculation of viewfactors) by setting the variable OMP_NUM_THREADS to the maximum number of cores on your system, and prevent parallelization of the material tangent and stress calculation step by setting CCX_NPROC_RESULTS to 1.

3 Units

An important issue which frequently raises questions concerns units. Finite element programs do not know any units. The user has to take care of that. In fact, there is only one golden rule: the user must make sure that the numbers he provides have consistent units. The number of units one can freely choose depends on the application. For thermomechanical problems you can choose

four units, e.g. for length, mass, time and temperature. If these are chosen, everything else is fixed. If you choose SI units for these quantities, i.e. m for length, kg for mass, s for time and K for temperature, force will be in $\mathrm{kgm/s^2}$ = N, pressure will be in $\mathrm{N/m^2}$ = $\mathrm{kg/ms^2}$, density will be in $\mathrm{kg/m^3}$, thermal conductivity in W/mK = J/smK = Nm/smK = $\mathrm{kgm^2/s^3mK}$ = $\mathrm{kgm/s^3K}$, specific heat in J/kgK = Nm/kgK = $\mathrm{m^2/s^2K}$ and so on. The density of steel in the SI system is 7800 $\mathrm{kg/m^3}$.

If you choose mm for length, g for mass, s for time and K for temperature, force will be in $\mathrm{gmm/s^2}$ and thermal conductivity in $\mathrm{gmm/s^3K}$. In the $\{\mathrm{mm, g, s, K}\}$ system the density of steel is 7.8×10^{-3} since $7800\mathrm{kg/m^3} = 7800 \times 10^{-6}\mathrm{g/mm^3}$.

However, you can also choose other quantities as the independent ones. A popular system at my company is mm for length, N for force, s for time and K for temperature. Now, since force = mass × length / $\mathrm{time^2}$, we get that mass = force × $\mathrm{time^2}$/length. This leads to $\mathrm{Ns^2/mm}$ for the mass and $\mathrm{Ns^2/mm^4}$ for density. This means that in the $\{\mathrm{mm, N, s, K}\}$ system the density of steel is 7.8×10^{-9} since $7800\mathrm{kg/m^3} = 7800\mathrm{Ns^2/m^4} = 7.8 \times 10^{-9}\mathrm{Ns^2/mm^4}$.

Notice that your are not totally free in choosing the four basic units: you cannot choose the unit of force, mass, length and time as basic units since they are linked with each other through force = mass × length / $\mathrm{time^2}$.

Finally, a couple of additional examples. Young's Modulus for steel is $210000\mathrm{N/mm^2} = 210000{\times}10^6\mathrm{N/m^2} = 210000{\times}10^6\mathrm{kg/ms^2} = 210000{\times}10^6\mathrm{g/mms^2}$. So its value in the SI system is 210×10^9, in the $\{\mathrm{mm, g, s, K}\}$ system it is also 210×10^9 and in the $\{\mathrm{mm, N, s, K}\}$ system it is 210×10^3. The heat capacity of steel is $446\mathrm{J/kgK} = 446\mathrm{m^2/s^2K} = 446 \times 10^6\mathrm{mm^2/s^2K}$, so in the SI system it is 446., in the $\{\mathrm{mm, g, s, K}\}$ and $\{\mathrm{mm, N, s, K}\}$ system it is 446×10^6.

Table 1 gives an overview of frequently used units in three different systems: the $\{\mathrm{m, kg, s, K}\}$ system, the $\{\mathrm{mm, N, s, K}\}$ system and the $\{\mathrm{cm, g, s, K}\}$ system.

4 Golden rules

Applying the finite element method to real-life problems is not always a piece of cake. Especially achieving convergence for nonlinear applications (large deformation, nonlinear material behavior, contact) can be quite tricky. However, adhering to a couple of simple rules can make life a lot easier. According to my experience, the following guidelines are quite helpful:

1. Check the quality of your mesh in CalculiX GraphiX or by using any other good preprocessor.

2. If you are dealing with a nonlinear problem, RUN A LINEARIZED VERSION FIRST: eliminate large deformations (drop NLGEOM), use a linear elastic material and drop all other nonlinearities such as contact. If the linear version doesn't run, the nonlinear problem won't run either. The linear version allows you to check easily whether the boundary conditions are correct (no unrestrained rigid body modes), the loading is the one

Table 1: Frequently used units in different unit systems.

symbol	meaning	m,kg,s,K	mm,N,s,K	cm,g,s,K
E	Young's Modulus	$1\frac{N}{m^2} = 1\frac{kg}{ms^2}$	$= 10^{-6}\frac{N}{mm^2}$	$= 1\frac{g}{mms^2}$
ρ	Density	$1\ \frac{kg}{m^3}$	$= 10^{-12}\frac{Ns^2}{mm^4}$	$= 10^{-6}\frac{g}{mm^3}$
F	Force	$1N = 1\frac{kgm}{s^2}$	$= 1N$	$= 10^{6}\frac{g\,mm}{s^2}$
c_p	Specific Heat	$1\frac{J}{kgK} = 1\frac{m^2}{s^2K}$	$= 10^{6}\frac{mm^2}{s^2K}$	$= 10^{6}\frac{mm^2}{s^2K}$
λ	Conductivity	$1\ \frac{W}{mK} = 1\frac{kgm}{s^3K}$	$= 1\frac{N}{sK}$	$= 10^{6}\frac{g\,mm}{s^3K}$
h	Film Coefficient	$1\frac{W}{m^2K} = 1\frac{kg}{s^3K}$	$= 10^{-3}\frac{N}{mm\,sK}$	$= 10^{3}\frac{g}{s^3K}$
μ	Dynamic Viscosity	$1\frac{Ns}{m^2} = 1\frac{kg}{ms}$	$= 10^{-6}\frac{Ns}{mm^2}$	$= 1\frac{g}{mm\,s}$

you meant to apply etc. Furthermore, you get a feeling what the solution should look like.

3. USE QUADRATIC ELEMENTS (C3D10, C3D15, C3D20(R), S8, CPE8, CPS8, CAX8, B32). The standard shape functions for quadratic elements are very good. Most finite element programs use these standard functions. For linear elements this is not the case: linear elements exhibit all kind of weird behavior such as shear locking and volumetric locking. Therefore, most finite element programs modify the standard shape functions for linear elements to alleviate these problems. However, there is no standard way of doing this, so each vendor has created his own modifications without necessarily publishing them. This leads to a larger variation in the results if you use linear elements. Since CalculiX uses the standard shape functions for linear elements too, the results must be considered with care.

4. If you are using shell elements or beam elements, use the option OUTPUT=3D on the *NODE FILE card in CalculiX (which is default). That way you get the expanded form of these elements in the .frd file. You can easily verify whether the thicknesses you specified are correct. Furthermore, you get the 3D stress distribution. It is the basis for the 1D/2D stress distribution and the internal beam forces. If the former is incorrect, so will the latter be.

5. If you include contact in your calculations and you are using quadratic ele-

ments, use the face-to-face penalty contact method. In general, for contact between faces the face-to-face penalty method will converge much better than the node-to-face method. The type of contact has to be declared on the *CONTACT PAIR card.

6. if you do not have enough space to run a problem, check the numbering. The memory needed to run a problem depends on the largest node and element numbers (the computational time, though, does not). So if you notice large gaps in the numbering, get rid of them and you will need less memory. In some problems you can save memory by choosing an iterative solution method. The iterative scaling method (cf. *STATIC) needs less memory than the iterative Cholesky method, the latter needs less memory than SPOOLES or PARDISO.

If you experience problems you can:

1. look at the screen output. In particular, the convergence information for nonlinear calculations may indicate the source of your problem.

2. look at the .sta file. This file contains information on the number of iterations needed in each increment to obtain convergence

3. look at the .cvg file. This file is a synopsis of the screen output: it gives you a very fast overview of the number of contact elements, the residual force and the largest change in solution in each iteration (no matter whether convergent or not).

4. use the “last iterations” option on the *NODE FILE or similar card. This generates a file with the name ResultsForLastIterations.frd with the deformation (for mechanical calculations) and the temperature (for thermal calculations) for all non-converged iterations starting after the last convergent increment.

5. if you have contact definitions in your input deck you may use the “contact elements” option on the *NODE FILE or similar card. This generates a file with the name “contactelements.inp” with all contact elements in all iterations of the increment in which this option is active. By reading this file in CalculiX GraphiX you can visualize all contact elements in each iteration and maybe find the source of your problems.

6. if you experience a segmentation fault, you may set the environment variable CCX_LOG_ALLOC to 1 by typing “export CCX_LOG_ALLOC=1” in a terminal window. Running CalculiX you will get information on which fields are allocated, reallocated or freed at which line in the code (default is 0).

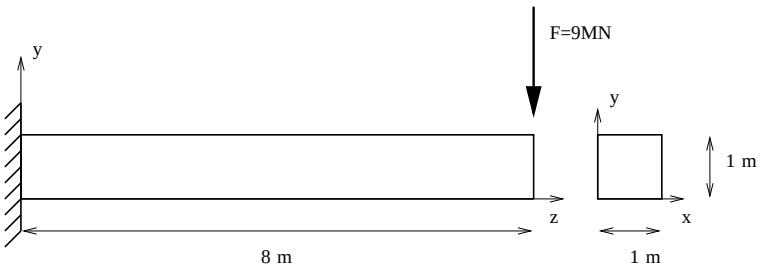


Figure 1: Geometry and boundary conditions of the beam problem

5 Simple example problems

5.1 Cantilever beam

In this section, a cantilever beam loaded by point forces at its free end is analyzed.

The geometry, loading and boundary conditions of the cantilever beam are shown in Figure 1. The size of the beam is 1x1x8 m^3, the loading consists of a point force of 9×10^6 N and the beam is completely fixed (in all directions) on the left end. Let us take 1 m and 1 MN as units of length and force, respectively. Assume that the beam geometry was generated and meshed with CalculiX GraphiX (cgx) resulting in the mesh in Figure 2. For reasons of clarity, only element labels are displayed.

A CalculiX input deck basically consists of a model definition section describing the geometry and boundary conditions of the problem and one or more steps (Figure 3) defining the loads.

The model definition section starts at the beginning of the file and ends at the occurrence of the first *STEP card. All input is preceded by keyword cards, which all start with an asterisk (*), indicating the kind of data which follows. *STEP is such a keyword card. Most keyword cards are either model definition cards (i.e. they can only occur before the first *STEP card) or step cards (i.e. they can only occur between *STEP and *END STEP cards). A few can be both.

In our example (Figure 4), the first keyword card is *HEADING, followed by a short description of the problem. This has no effect on the output and only serves for identification. Then, the coordinates are given as triplets preceded by the *NODE keyword. Notice that data on the same line are separated by commas and must not exceed a record length of 132 columns. A keyword card can be repeated as often as needed. For instance, each node could have been preceded by its own *NODE keyword card.

Next, the topology is defined by use of the keyword card *ELEMENT. Defining the topology means listing for each element its type, which nodes belong to the element and in what order. The element type is a parameter on the keyword card. In the beam case 20-node brick elements with reduced integration have

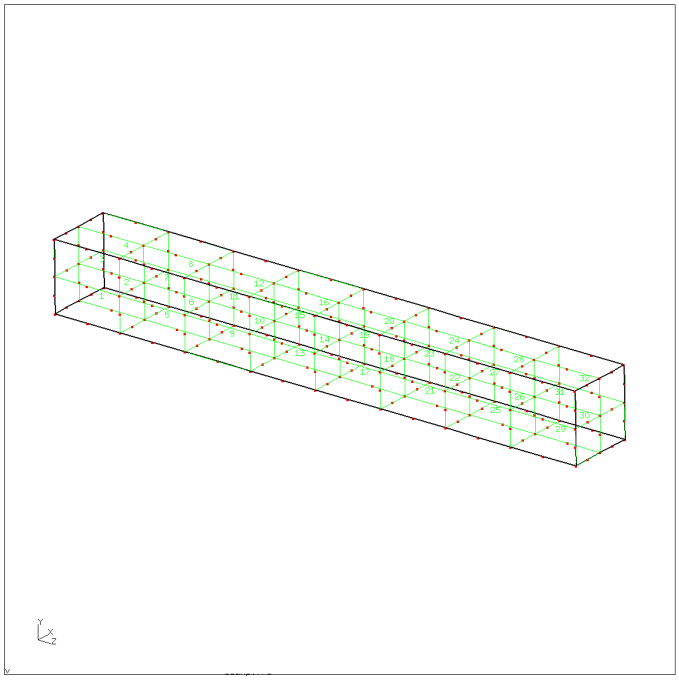


Figure 2: Mesh for the beam

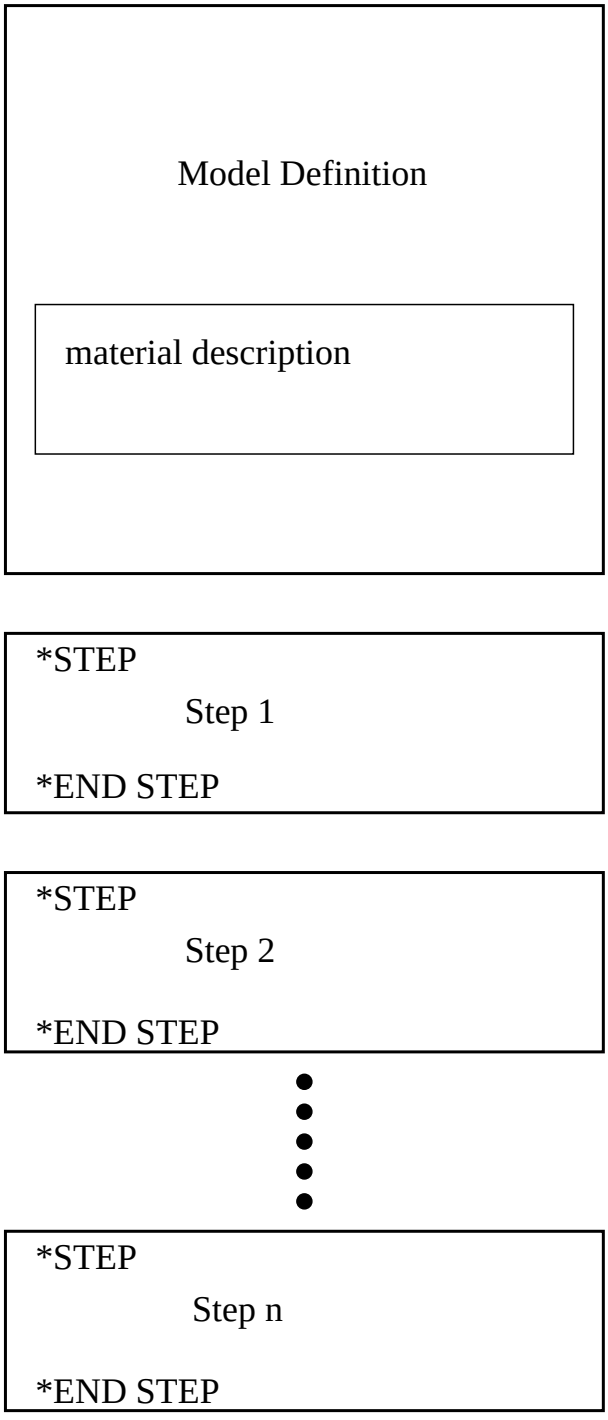


Figure 3: Structure of a CalculiX input deck

```
*HEADING
Model: beam     Date: 10-Mar-1998
*NODE
     1,      0.000000,      0.000000,      0.000000
     2,      1.000000,      0.000000,      0.000000
     3,      1.000000,      1.000000,      0.000000
     .
     .
     .
   260,      0.500000,      0.750000,      7.000000
   261,      0.500000,      0.500000,      7.500000
*ELEMENT, TYPE=C3D20R   , ELSET=Eall
     1,     1,    10,    95,    19,    61,   105,   222,   192,     9,    93,
           94,    20,   104,   220,   221,   193,    62,   103,   219,   190
     2,    10,     2,    13,    95,   105,    34,   134,   222,    11,    12,
           96,    93,   106,   133,   223,   220,   103,    33,   132,   219
     .
     .
     .
     .
    32,   258,   158,    76,   187,   100,    25,     7,    28,   259,   159,
          186,   260,   101,    26,    27,   102,   261,   160,    77,   189
*NSET, NSET=FIX
    97,    96,    95,    94,    93,    20,    19,    18,    17,    16,    15,
    14,    13,    12,    11,    10,     9,     4,     3,     2,     1
*BOUNDARY
FIX, 1
*BOUNDARY
FIX, 2
*BOUNDARY
FIX, 3
*NSET,NSET=Nall,GENERATE
1,261
*MATERIAL,NAME=EL
*ELASTIC
  210000.0,        .3
*SOLID SECTION,ELSET=Eall,MATERIAL=EL
*NSET,NSET=LOAD
5,6,7,8,22,25,28,31,100
**
*STEP
*STATIC
*CLOAD
LOAD,2,1.
*NODE PRINT,NSET=Nall
U
*EL PRINT,ELSET=Eall
S
*NODE FILE
U
*EL FILE
S
*END STEP
```

Figure 4: Beam input deck

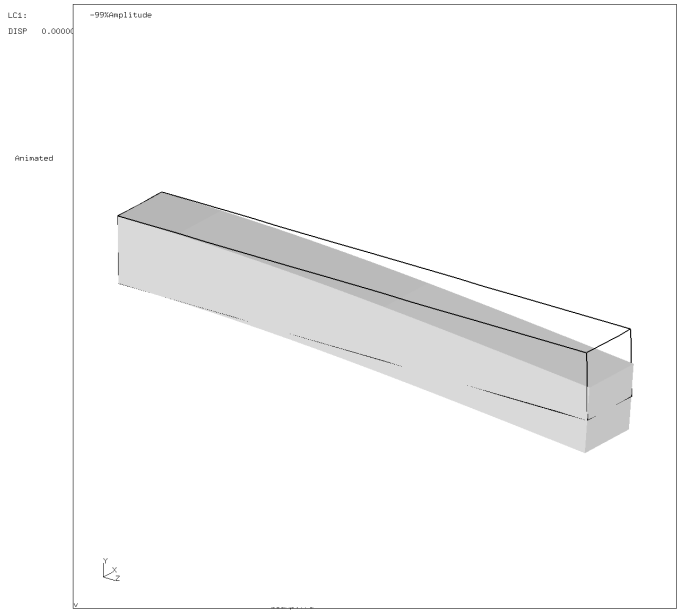


Figure 5: Deformation of the beam

been used, abbreviated as C3D20R. In addition, by adding ELSET=Eall, all elements following the *ELEMENT card are stored in set Eall. This set will be later referred to in the material definition. Now, each element is listed followed by the 20 node numbers defining it. With *NODE and *ELEMENT, the core of the geometry description is finished. Remaining model definition items are geometric boundary conditions and the material description.

The only geometric boundary condition in the beam problem is the fixation at z=0. To this end, the nodes at z=0 are collected and stored in node set FIX defined by the keyword card *NSET. The nodes belonging to the set follow on the lines underneath the keyword card. By means of the card *BOUNDARY, the nodes belonging to set FIX are subsequently fixed in 1, 2 and 3-direction, corresponding to x,y and z. The three *BOUNDARY statements in Figure 4 can actually be grouped yielding:

```
*BOUNDARY
FIX,1
FIX,2
FIX,3
```

or even shorter:

```
*BOUNDARY
FIX,1,3
```

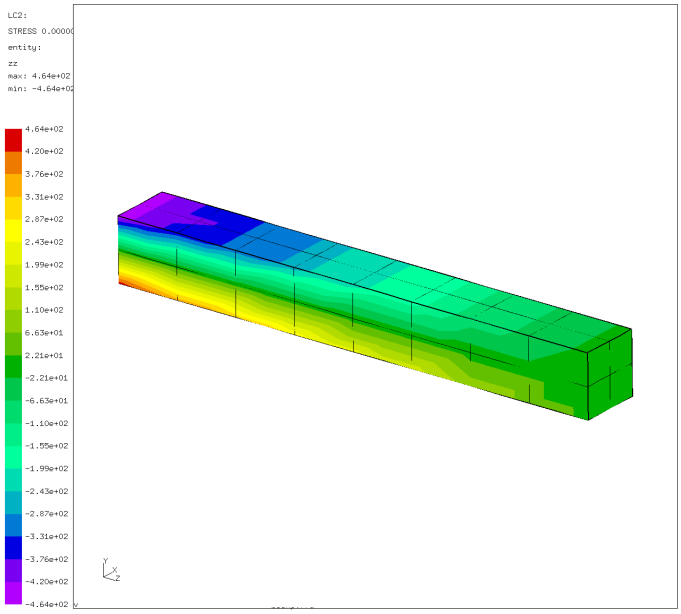


Figure 6: Axial normal stresses in the beam

meaning that degrees of freedom 1 through 3 are to be fixed (i.e. set to zero).

The next section in the input deck is the material description. This section is special since the cards describing one and the same material must be grouped together, although the section itself can occur anywhere before the first *STEP card. A material section is always started by a *MATERIAL card defining the name of the material by means of the parameter NAME. Depending on the kind of material several keyword cards can follow. Here, the material is linear elastic, characterized by a Young's modulus of 210,000.0 MN/m^2 and a Poisson coefficient of 0.3 (steel). These properties are stored beneath the *ELASTIC keyword card, which here concludes the material definition. Next, the material is assigned to the element set Eall by means of the keyword card *SOLID SECTION.

Finally, the last card in the model definition section defines a node set LOAD which will be needed to define the load. The card starting with two asterisks in between the model definition section and the first step section is a comment line. A comment line can be introduced at any place. It is completely ignored by CalculiX and serves for input deck clarity only.

In the present problem, only one step is needed. A step always starts with a *STEP card and concludes with a *END STEP card. The keyword card *STATIC defines the procedure. The *STATIC card indicates that the load is applied in a quasi-static way, i.e. so slow that mass inertia does not play a

role. Other procedures are *FREQUENCY, *BUCKLE, *MODAL DYNAMIC, *STEADY STATE DYNAMICS and *DYNAMIC. Next, the concentrated load is applied (keyword *CLOAD) to node set LOAD. The forces act in y-direction and their magnitude is 1, yielding a total load of 9.

Finally, the printing and file storage cards allow for user-directed output generation. The print cards (*NODE PRINT and *EL PRINT) lead to an ASCII file with extension .dat. If they are not selected, no .dat file is generated. The *NODE PRINT and *EL PRINT cards must be followed by the node and element sets for which output is required, respectively. Element information is stored at the integration points.

The *NODE FILE and *EL FILE cards, on the other hand, govern the output written to an ASCII file with extension .frd. The results in this file can be viewed with CalculiX GraphiX (cgx). Quantities selected by the *NODE FILE and *EL FILE cards are always stored for the complete model. Element quantities are extrapolated to the nodes, and all contributions in the same node are averaged. Selection of fields for the *NODE PRINT, *EL PRINT, *NODE FILE and *EL FILE cards is made by character codes: for instance, U are the displacements and S are the (Cauchy) stresses.

The input deck is concluded with an *END STEP card.

The output files for the beam problem consist of file beam.dat and beam.frd. The beam.dat file contains the displacements for set Nall and the stresses in the integration points for set Eall. The file beam.frd contains the displacements and extrapolated stresses in all nodes. It is the input for the visualization program CalculiX GraphiX (cgx). An impression of the capabilities of cgx can be obtained by looking at Figures 5, 6 and 7.

Figure 5 shows the deformation of the beam under the prevailing loads. As expected, the beam bends due to the lateral force at its end. Figure 6 shows the normal stress in axial direction. Due to the bending moment one obtains a nearly linear distribution across the height of the beam. Finally, Figure 7 shows the Von Mises stress in the beam.

5.2 Frequency calculation of a beam loaded by compressive forces

Let us consider the beam from the previous section and determine its eigenfrequencies and eigenmodes. To obtain different frequencies for the lateral directions the cross section is changed from 1x1 to 1x1.5. Its length is kept (8 length units). The input deck is very similar to the one in the previous section, Figure 8. The full deck is part of the test example suite (beamf2.inp).

The only significant differences relate to the steps. In the first step the preload is applied in the form of compressive forces at the end of the beam. In each node belonging to set LAST a compressive force is applied with a value of -48.155 in the positive z-direction, or, which is equivalent, with magnitude 48.155 in the negative z-direction. The second step is a frequency step. By using the parameter PERTURBATION on the *STEP keyword card the user specifies that the deformation and stress from the previous static step should be taken

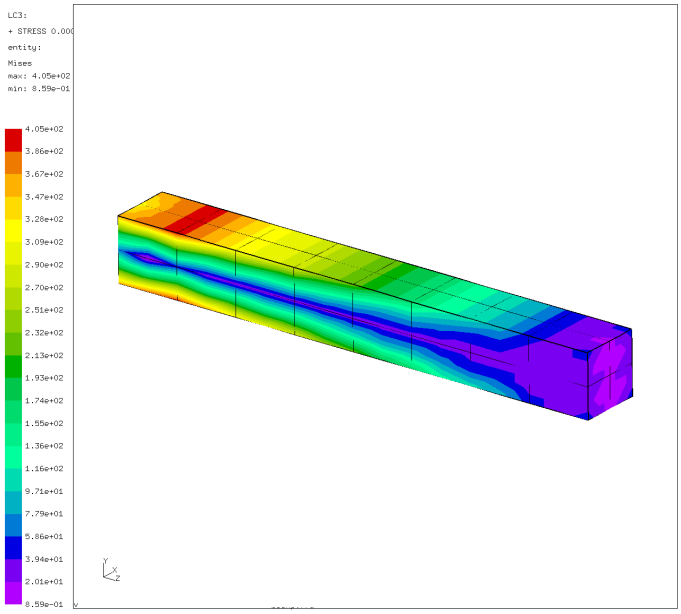


Figure 7: Von Mises stresses in the beam

into account in the subsequent frequency calculation. The *FREQUENCY card and the line underneath indicate that this is a modal analysis step and that the 10 lowest eigenfrequencies are to be determined. They are automatically stored in the .dat file. Table 2 shows these eigenfrequencies for the beam without and with preload together with a comparison with ABAQUS (the input deck for the modal analysis without preload is stored in file beamf.inp of the test example suite). One notices that due to the preload the eigenfrequencies drop. This is especially outspoken for the lower frequencies. As a matter of fact, the lowest bending eigenfrequency is so low that buckling will occur. Indeed, one way of determining the buckling load is by increasing the compressive load up to the point that the lowest eigenfrequency is zero. For the present example this means that the buckling load is 21 x 48.155 = 1011.3 force units (the factor 21 stems from the fact that the same load is applied in 21 nodes). An alternative way of determining the buckling load is to use the *BUCKLE keyword card. This is illustrated for the same beam geometry in file beamb.inp of the test suite.

Figures 9 and 10 show the deformation of the second bending mode across the minor axis of inertia and deformation of the first torsion mode.

```
**
**   Structure: beam under compressive forces.
**   Test objective: Frequency analysis; the forces are that
**                   high that the lowest frequency is nearly
**                   zero, i.e. the buckling load is reached.
**
*HEADING
Model: beam     Date: 10-Mar-1998
*NODE
     1,      0.000000,      0.000000,      0.000000
     .
     .
*ELEMENT, TYPE=C3D20R
     1,     1,    10,    95,    19,    61,   105,   222,   192,     9,    93,
           94,    20,   104,   220,   221,   193,    62,   103,   219,   190
     .
     .
*NSET, NSET=CN7
    97,    96,    95,    94,    93,    20,    19,    18,    17,    16,    15,
    14,    13,    12,    11,    10,     9,     4,     3,     2,     1
*BOUNDARY
CN7, 1
*BOUNDARY
CN7, 2
*BOUNDARY
CN7, 3
*ELSET,ELSET=EALL,GENERATE
1,32
*MATERIAL,NAME=EL
*ELASTIC
  210000.0,        .3
*DENSITY
7.8E-9
*SOLID SECTION,MATERIAL=EL,ELSET=EALL
*NSET,NSET=LAST
     5,
     6,
     .
     .
*STEP
*STATIC
*CLOAD
LAST,3,-48.155
*END STEP
*STEP,PERTURBATION
*FREQUENCY
10
*NODE FILE
U
*EL FILE
S
*END STEP
```

Figure 8: Frequency input deck

Table 2: Frequencies without and with preload (cycles/s).

without preload		with preload	
CalculiX	ABAQUS	CalculiX	ABAQUS
13,096.	13,096.	705.	1,780.
19,320.	19,319.	14,614.	14,822.
76,840.	76,834.	69,731.	70,411.
86,955.	86,954.	86,544.	86,870.
105,964.	105,956.	101,291.	102,148.
162,999.	162,998.	162,209.	163,668.
197,645.	197,540.	191,581.	193,065.
256,161.	256,029.	251,858.	253,603.
261,140.	261,086.	259,905.	260,837.
351,862.	351,197.	345,729.	347,688.

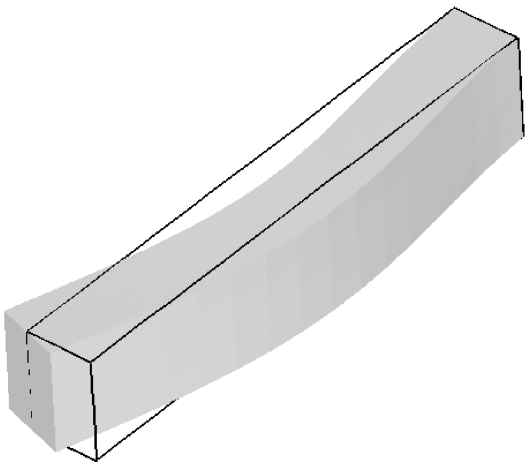


Figure 9: Second bending mode across the minor axis of inertia

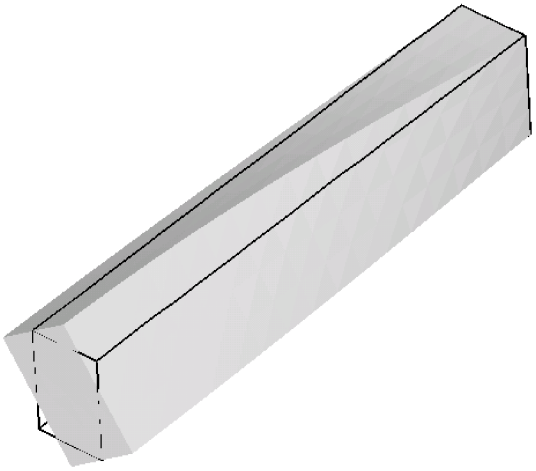


Figure 10: First torsion mode

5.3 Frequency calculation of a rotating disk on a slender shaft

This is an example for a complex frequency calculation. A disk with an outer diameter of 10, an inner diameter of 2 and a thickness of 0.25 is mounted on a hollow shaft with outer diamter 2 and inner diameter 1 (example rotor.inp in het test examples). The disk is mounted in het middle of the shaft, the ends of which are fixed in all directions. The length of the shaft on either side of the disk is 50. The input deck for this example is shown in Figure 11.

The deck start with the definition of the nodes and elements. The set Nfix contains the nodes at the end of the shaft, which are fixed in all directions. The material is ordinary steel. Notice that the density is needed for the centrifugal loading.

Since the disk is rotation there is a preload in the form of centrifugal forces. Therefore, the first step is a nonlinear geometric static step in order to calculate the deformation and stresses due to this loading. By selecting the parameter perturbation in the subsequent frequency step this preload is taken into account in the calculation of the stiffness matrix in the frequency calculation. The resulting eigenfrequencies are stored at the top of file rotor.dat (Figure 12 for a rotational speed of 9000 rad/s). In a *FREQUENCY step an eigenvalue problem is solved, the eigenvalues of which (first column on the top of Figure 12) are the square of the eigenfrequencies of the structure (second to fourth column). If the eigenvalue is negative, an imaginary eigenfrequency results. This is the case for the two lowest eigenvalues for the rotor rotating at 9000 rad/s. For shaft

```
**
**   Structure: slender disk mounted on a long shaft
**   Test objective: *COMPLEX FREQUENCY.
**
*NODE, NSET=Nall
       1,6.123233995737e-17,1.000000000000e+00,0.000000000000e+00
        ...
*ELEMENT, TYPE=C3D20R, ELSET=Eall
     1,      1,      2,      3,      4,      5,      6,      7,      8,      9,     10,
          11,     12,     17,     18,     19,     20,     13,     14,     15,     16
     ...
*NSET,NSET=Nfix
14,
136,
...
*BOUNDARY
Nfix,1,3
*Solid Section, elset=Eall, material=steel
*Material, name=STEEL
*Elastic
 210000., 0.3
*DENSITY
7.8e-9
*Step,nlgeom
*Static
*dload
Eall,centrif,3.0853e8,0.,0.,0.,0.,0.,1.
*end step
*step,perturbation
*frequency,STORAGE=YES
 10,
*end step
*step
*complex frequency
 10,
*NODE FILE
PU
*end step
```

Figure 11: Input deck for the rotor

E I G E N V A L U E O U T P U T

MODE NO	EIGENVALUE	FREQUENCY		
		REAL PART (RAD/TIME)	(CYCLES/TIME	IMAGINARY PART (RAD/TIME)
1	-0.4710377E+08	0.0000000E+00	0.0000000E+00	0.6863218E+04
2	-0.4710377E+08	0.0000000E+00	0.0000000E+00	0.6863218E+04
3	0.2240062E+09	0.1496684E+05	0.2382046E+04	0.0000000E+00
4	0.2240062E+09	0.1496684E+05	0.2382046E+04	0.0000000E+00
5	0.9466374E+09	0.3076747E+05	0.4896795E+04	0.0000000E+00
6	0.9466374E+09	0.3076747E+05	0.4896795E+04	0.0000000E+00
7	0.2028547E+10	0.4503940E+05	0.7168243E+04	0.0000000E+00
8	0.2930439E+10	0.5413353E+05	0.8615618E+04	0.0000000E+00
9	0.2930439E+10	0.5413353E+05	0.8615618E+04	0.0000000E+00
10	0.5367484E+10	0.7326312E+05	0.1166019E+05	0.0000000E+00

E I G E N V A L U E O U T P U T

MODE NO	FREQUENCY		
	REAL PART (RAD/TIME)	(CYCLES/TIME)	IMAGINARY PART (RAD/TIME)
1	0.3179491E+04	0.5060316E+03	0.3031618E-03
2	0.8499901E+04	0.1352801E+04	-0.2864205E-04
3	0.1481488E+05	0.2357861E+04	-0.1108269E-02
4	0.2307301E+05	0.3672184E+04	-0.3240550E-04
5	0.2634670E+05	0.4193207E+04	0.1973187E-04
6	0.4102791E+05	0.6529794E+04	0.8690869E-04
7	0.4503940E+05	0.7168244E+04	0.2343947E-06
8	0.4649931E+05	0.7400595E+04	0.6623206E-04
9	0.6262165E+05	0.9966545E+04	0.5469548E-04
10	0.7375084E+05	0.1173781E+05	0.2650943E-05

Figure 12: Eigenfrequencies for the rotor

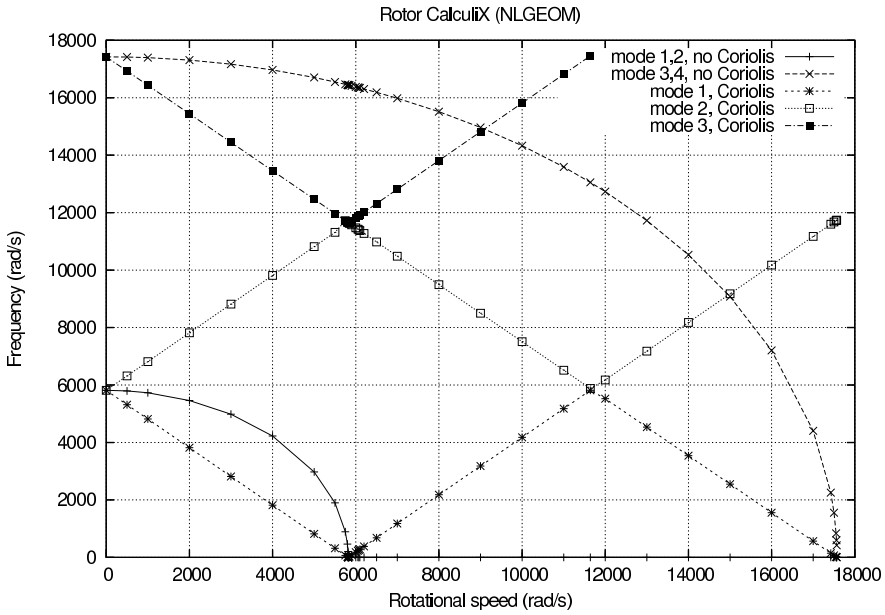


Figure 13: Eigenfrequencies as a function of shaft speed

speeds underneath about 6000 rad/s all eigenfrequencies are real. The lowest eigenfrequencies as a function of rotating speeds up to 18000 rad/s are shown in Figure 13 (+ and x curves).

What is the physical meaning of imaginary eigenfrequencies? The eigenmodes resulting from a frequency calculation contain the term $e^{i\omega t}$. If the eigenfrequency ω is real, one obtains a sine or cosine, if ω is imaginary, one obtains an increasing or decreasing exponential function [18]. Thus, for imaginary eigenfrequencies the response is not any more oscillatory: it increases indefinitely, the system breaks apart. Looking at Figure 13 one observes that the lowest eigenfrequency decreases for increasing shaft speed up to the point where it is about zero at a shaft speed of nearly 6000 rad/s. At that point the eigenfrequency becomes imaginary, the rotor breaks apart. This has puzzled engineers for a long time, since real systems were observed to reach supercritical speeds without breaking apart.

The essential point here is to observe that the calculations are being performed in a rotating coordinate system (fixed to the shaft). Newton's laws are not valid in an accelerating reference system, and a rotating coordinate system is accelerating. A correction term to Newton's laws is necessary in the form of a Coriolis force. The introduction of the Coriolis force leads to a complex nonlinear eigenvalue system, which can solved with the *COMPLEX FREQUENCY procedure (cf. Section 6.9.3). One can prove that the resulting eigenfrequencies are real, the eigenmodes, however, are usually complex. This leads to rotating eigenmodes.

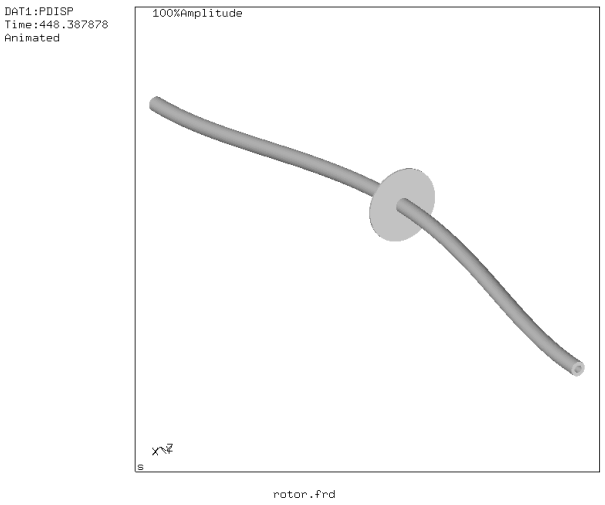


Figure 14: Two-node eigenmode

In order to use the *COMPLEX FREQUENCY procedure the eigenmodes without Coriolis force must have been calculated and stored in a previous *FREQUENCY step (STORAGE=YES) (cf. Figure 11). The complex frequency response is calculated as a linear combination of these eigenmodes. The number of eigenfrequencies requested in the *COMPLEX FREQUENCY step should not exceed those of the preceding *FREQUENCY step. Since the eigenmodes are complex, they are best stored in terms of amplitude and phase with PU underneath the *NODE FILE card.

The correct eigenvalues for the rotating shaft lead to the straight lines in Figure 13. Each line represents an eigenmode: the lowest decreasing line is a two-node counter clockwise (ccw) eigenmode when looking in (-z)-direction, the highest decreasing line is a three-node ccw eigenmode, the lowest and highest increasing lines constitute both a two-node clockwise (cw) eigenmode. A node is a location at which the radial motion is zero. Figure 14 shows the two-node eigenmode, Figure 15 the three-node eigenmode. Notice that if the scales on the x- and y-axis in Figure 13 were the same the lines would be under 45°.

It might surprise that both increasing straight lines correspond to one and the same eigenmode. For instance, for a shaft speed of 5816 rad/s one and the same eigenmode occurs at an eigenfrequency of 0 and 11632 rad/s. Remember, however, that the eigenmodes are calculated in the rotating system, i.e. as observed by an observer rotating with the shaft. To obtain the frequencies for a fixed observer the frequencies have to be considered relative to a 45° straight line through the origin and bisecting the diagram. This observer will see one and the same eigenmode at 5816 rad/s and -5816 rad/s, so cw and ccw.

Finally, the Coriolis effect is not always relevant. Generally, slender rotating structures (large blades...) will exhibit important frequency shifts due to

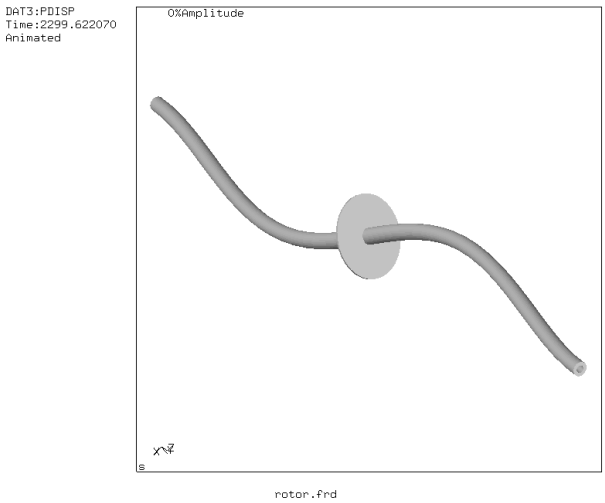


Figure 15: Three-node eigenmode

Coriolis.

5.4 Thermal calculation of a furnace

This problem involves a thermal calculation of the furnace depicted in Figure 16. The furnace consists of a bottom plate at a temperature Tb, which is prescribed. It changes linearly in an extremely short time from 300 K to 1000 K after which it remains constant. The side walls of the furnace are isolated from the outer world, but exchange heat through radiation with the other walls of the furnace. The emissivity of the side walls and bottom is $\epsilon = 1$. The top of the furnace exchanges heat through radiation with the other walls and with the environmental temperature which is fixed at 300 K. The emissivity of the top is $\epsilon = 0.8$. Furthermore, the top exchanges heat through convection with a fluid (air) moving at the constant rate of 0.001 kg/s. The temperature of the fluid at the right upper corner is 300 K. The walls of the oven are made of 10 cm steel. The material constants for steels are: heat conductivity $\kappa = 50\text{W/mK}$, specific heat $c = 446\text{W/kgK}$ and density $\rho = 7800\text{kg/m}^3$. The material constants for air are : specific heat $c_p = 1000\text{W/kgK}$ and density $\rho = 1\text{kg/m}^3$. The convection coefficient is $h = 25\text{W/m}^2\text{K}$. The dimensions of the furnace are $0.3 \times 0.3 \times 0.3\text{m}^3$ (cube). At $t = 0$ all parts are at $T = 300\text{K}$. We would like to know the temperature at locations A,B,C,D and E as a function of time.

The input deck is listed in Figure 17. It starts with the node definitions. The highest node number in the structure is 602. The nodes 603 up to 608 are fluid nodes, i.e. in the fluid extra nodes were defined (z=0.3 corresponds with the top of the furnace, z=0 with the bottom). Fluid node 603 corresponds to the location where the fluid temperature is 300 K (“inlet”), node 608 corresponds

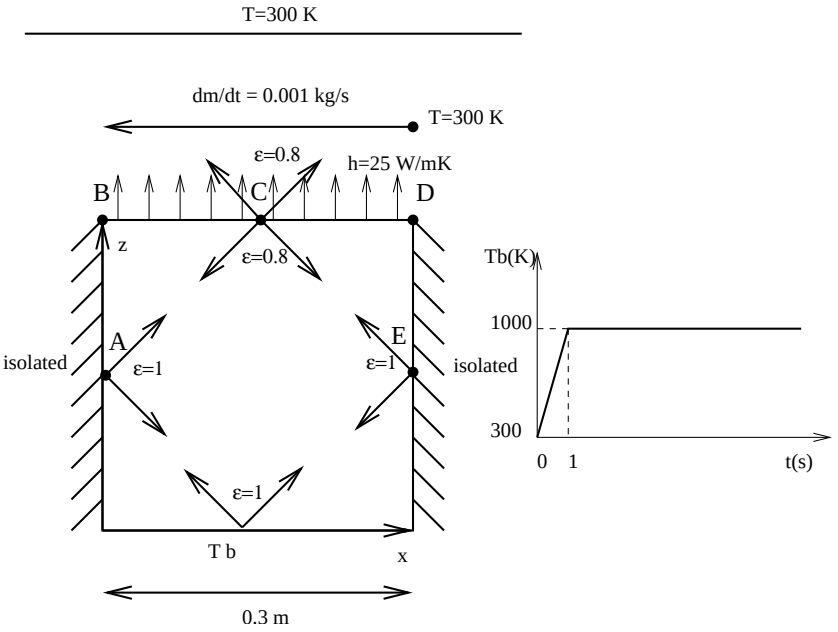


Figure 16: Description of the furnace

to the "outlet", the other nodes are located in between. The coordinates of the fluid nodes actually do not enter the calculations. Only the convective definitions with the keyword *FILM govern the exchange between furnace and fluid. With the *ELEMENT card the 6-node shell elements making up the furnace walls are defined. Furthermore, the fluid nodes are also assigned to elements (element type D), so-called network elements. These elements are needed for the assignment of material properties to the fluid. Indeed, traditionally material properties are assigned to elements and not to nodes. Each network element consists of two end nodes, in which the temperature is unknown, and a midside node, which is used to define the mass flow rate through the element. The fluid nodes 603 up to 613 are assigned to the network elements 301 up to 305.

Next, two node sets are defined: GAS contains all fluid nodes, Ndown contains all nodes on the bottom of the furnace.

The *PHYSICAL CONSTANTS card is needed in those analyses in which radiation plays a role. It defines absolute zero, here 0 since we work in Kelvin, and the Stefan Boltzmann constant. In the present input deck SI units are used throughout.

Next, the material constants for STEEL are defined. For thermal analyses the conductivity, specific heat and density must be defined. The *SHELL SECTION card assigns the STEEL material to the element set FURNACE, defined by the *ELEMENT statement before. It contains all elements belonging to the furnace. Furthermore, a thickness of 0.01 m is assigned.

```
furnace.txt       Sun Feb 12 13:12:10 2006       1
*NODE, NSET=Nall
       1,  3.00000e-01,  3.72529e-09,  3.72529e-09
...
603,-0.1,0.5,1.
...
613,0.8,0.5,1.
*ELEMENT, TYPE=S6, ELSET=furnace
     1,      1,      2,      3,      4,      5,      6
...
*ELEMENT,TYPE=D,ELSET=EGAS
301,603,609,604
...
305,607,613,608
*NSET,NSET=NGAS,GENERATE
603,608
*NSET,NSET=Ndown
1,
...
*PHYSICAL CONSTANTS,ABSOLUTE ZERO=0.,STEFAN BOLTZMANN=5.669E-8
*MATERIAL,NAME=STEEL
*DENSITY
7800.
*CONDUCTIVITY
50.
*SPECIFIC HEAT
446.
*SHELL SECTION,ELSET=furnace,MATERIAL=STEEL
0.01
*MATERIAL,NAME=GAS
*DENSITY
1.
*SPECIFIC HEAT
1000.
*FLUID SECTION,ELSET=EGAS,MATERIAL=GAS
*INITIAL CONDITIONS,TYPE=TEMPERATURE
Nall,300.
*AMPLITUDE,NAME=A1
0.,.3,1.,1.
*STEP,INC=100
*HEAT TRANSFER
0.1,1.
*BOUNDARY,AMPLITUDE=A1
Ndown,11,11,1000.
*BOUNDARY
603,11,11,300.
*BOUNDARY
609,1,1,0.001
...
*RADIATE
** Radiate based on down
1, R1CR,1000., 1.000000e+00
...
** Radiate based on top
51, R1CR, 1000.000000, 8.000000e-01
...
** Radiate based on side
101, R1CR, 1000.000000, 1.
...
** Radiate based on top
51, R2, 300.000000, 8.000000e-01
...
*FILM
51, F2FC, 604, 2.500000e+01
...
*NODE FILE
NT
*NODE PRINT,NSET=NGAS
NT
*END STEP
```

Figure 17: Input deck for the furnace

The material constants for material GAS consist of the density and the specific heat. These are the constants for the fluid. Conduction in the fluid is not considered. The material GAS is assigned to element set EGAS containing all network elements.

The *INITIAL CONDITIONS card defines an initial temperature of 300 K for all nodes, i.e. furnace nodes AND fluid nodes. The *AMPLITUDE card defines a ramp function starting at 0.3 at 0.0 and increasing linearly to 1.0 at 1.0. It will be used to define the temperature boundary conditions at the bottom of the furnace. This ends the model definition.

The first step describes the linear increase of the temperature boundary condition between $t = 0$ and $t = 1$. The INC=100 parameter on the *STEP card allows for 100 increments in this step. The procedure is *HEAT TRANSFER, i.e. we would like to perform a purely thermal analysis: the only unknowns are the temperature and there are no mechanical unknowns (e.g. displacements). The step time is 1., the initial increment size is 0.1. Both appear on the line underneath the *HEAT TRANSFER card. The absence of the parameter STEADY STATE on the *HEAT TRANSFER card indicates that this is a transient analysis.

Next come the temperature boundary conditions: the bottom plate of the furnace is kept at 1000 K, but is modulated by amplitude A1. The result is that the temperature boundary condition starts at 0.3 x 1000 = 300K and increases linearly to reach 1000 K at t=1 s. The second boundary conditions specifies that the temperature of (fluid) node 603 is kept at 300 K. This is the inlet temperature. Notice that "11" is the temperature degree of freedom.

The mass flow rate in the fluid is defined with the *BOUNDARY card applied to the first degree of freedom of the midside nodes of the network elements. The first line tells us that the mass flow rate in (fluid)node 609 is 0.001. Node 609 is the midside node of network element 301. Since this rate is positive the fluid flows from node 603 towards node 604, i.e. from the first node of network element 301 to the third node. The user must assure conservation of mass (this is actually also checked by the program).

The first set of radiation boundary conditions specifies that the top face of the bottom of the furnace radiates through cavity radiation with an emissivity of 1 and an environment temperature of 1000 K. For cavity radiation the environment temperature is used in case the viewfactor at some location does not amount to 1. What is short of 1 radiates towards the environment. The first number in each line is the element, the number in the label (the second entry in each line) is the face of the element exposed to radiation. In general, these lines are generated automatically in cgx (CalculiX GraphiX).

The second and third block define the internal cavity radiation in the furnace for the top and the sides. The fourth block defines the radiation of the top face of the top plate of the furnace towards the environment, which is kept at 300 K. The emissivity of the top plate is 0.8.

Next come the film conditions. Forced convection is defined for the top face of the top plate of the furnace with a convection coefficient $h = 25\text{W/mK}$. The first line underneath the *FILM keyword indicates that the second face of

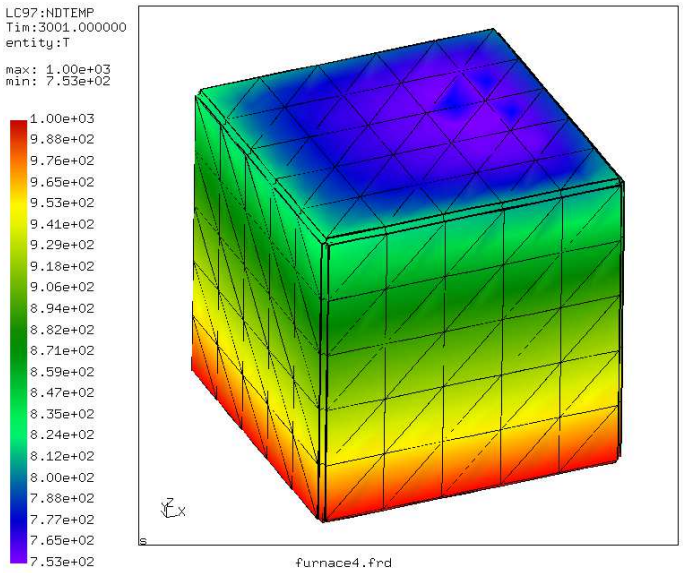


Figure 18: Temperature distribution at t=3001 s

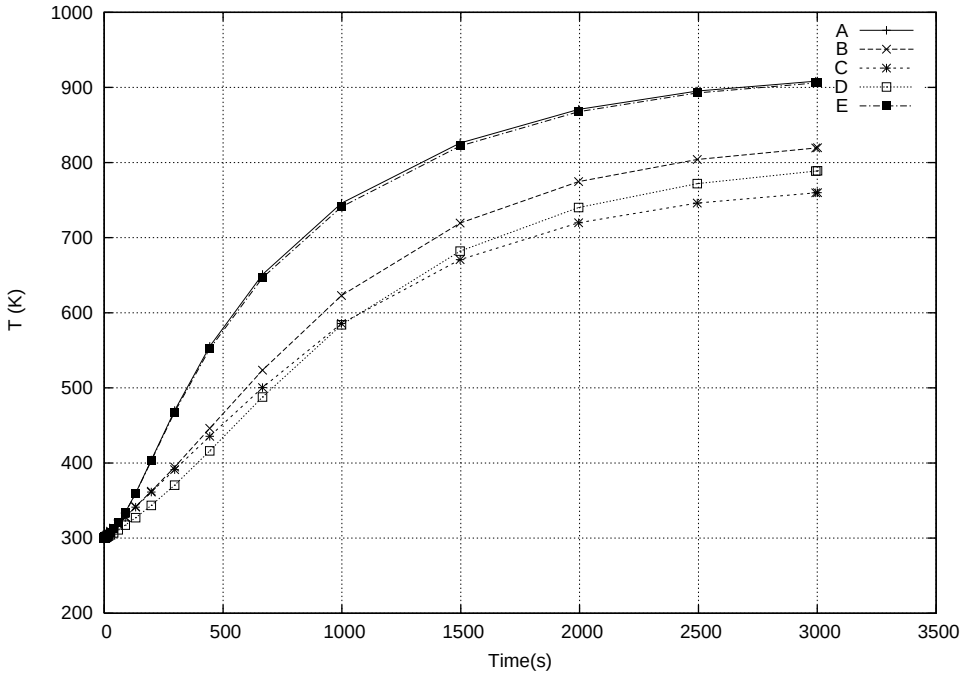


Figure 19: Temperature at selected positions

element 51 interacts through forced convection with (fluid)node 604. The last entry in this line is the convection coefficient. So for each face interacting with the fluid an appropriate fluid node must be specified with which the interaction takes place.

Finally, the *NODE FILE card makes sure that the temperature is stored in the .frd file and the *NODE PRINT card takes care that the fluid temperature is stored in the .dat file.

The complete input deck is part of the test examples of CalculiX (furnace.inp). For the present analysis a second step was appended keeping the bottom temperature constant for an additional 3000 seconds.

What happens during the calculation? The walls and top of the furnace heat up due to conduction in the walls and radiation from the bottom. However, the top of the furnace also loses heat through radiation with the environment and convection with the fluid. Due to the interaction with the fluid the temperature is asymmetric: at the inlet the fluid is cool and the furnace will lose more heat than at the outlet, where the temperature of the fluid is higher and the temperature difference with the furnace is smaller. So due to convection we expect a temperature increase from inlet to outlet. Due to conduction we expect a temperature minimum in the middle of the top. Both effects are superimposed. The temperature distribution at $t = 3001$s is shown in Figure 18. There is a temperature gradient from the bottom of the furnace towards the top. At the top the temperature is indeed not symmetric. This is also shown in Figure 19, where the temperature of locations A, B, C, D and E is plotted as a function of time.

Notice that steady state conditions have not been reached yet. Also note that 2D elements (such as shell elements) are automatically expanded into 3D elements with the right thickness. Therefore, the pictures, which were plotted from within CalculiX GraphiX, show 3D elements.

5.5 Seepage under a dam

In this section, groundwater flow under a dam is analyzed. The geometry of the dam is depicted in Figure 20 and is taken from exercise 30 in Chapter 1 of [27]. All length measurements are in feet (0.3048 m). The water level upstream of the dam is 20 feet high, on the downstream side it is 5 feet high. The soil underneath the dam is anisotropic. Upstream the permeability is characterized by $k_1 = 4k_2 = 10^{-2}$cm/s, downstream we have $25k_3 = 100k_4 = 10^{-2}$cm/s. Our primary interest is the hydraulic gradient, i.e. ∇h since this is a measure whether or not piping will occur. Piping means that the soil is being carried away by the groundwater flow (usually at the downstream side) and constitutes an instable condition. As a rule of thumb, piping will occur if the hydraulic gradient is about unity.

From Section 6.9.14 we know that the equations governing stationary groundwater flow are the same as the heat equations. The equivalent quantity of the total head is the temperature and of the velocity it is the heat flow. For the finite element analysis SI units were taken, so feet was converted into meter.

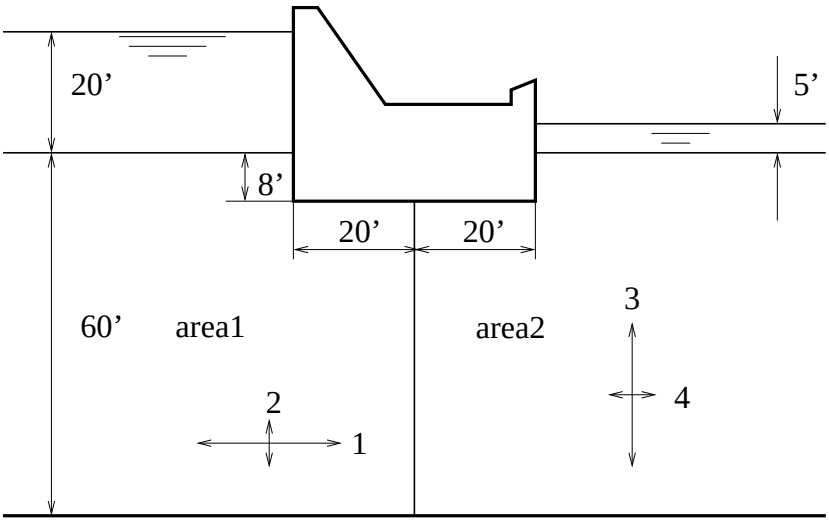


Figure 20: Geometry of the dam

Furthermore, a vertical impermeable wall was assumed far upstream and far downstream (actually, 30 m upstream from the middle point of the dam and 30 m downstream).

Now, the boundary conditions are:

1. the dam, the left and right vertical boundaries upstream and downstream, and the horizontal limit at the bottom are impermeable. This means that the water velocity perpendicular to these boundaries is zero, or, equivalently, the heat flux.

2. taking the reference for the z-coordinate in the definition of total head at the bottom of the dam (see Equation 221 for the definition of total head), and assuming that the atmospheric pressure p_0 is zero, the total head upstream is 28 feet and downstream it is 13 feet. In the thermal equivalent this corresponds to temperature boundary conditions.

The input deck is summarized in Figure 21. The complete deck is part of the example problems. The problem is really two-dimensional and consequently qu8 elements were used for the mesh generation within CalculiX GraphiX. To obtain a higher resolution immediately adjacent to the dam a bias was used (the mesh can be seen in Figure 22).

At the start of the deck the nodes are defined and the topology of the elements. The qu8 element type in CalculiX GraphiX is by default translated by the send command into a S8 (shell) element in CalculiX CrunchiX. However, a plane element is here more appropriate. Since the calculation at stake is thermal and not mechanical, it is really immaterial whether one takes plane strain (CPE8) or plane stress (CPS8) elements. With the *ELSET keyword

```
dam.txt       Sun Feb 12 13:17:58 2006       1
**
**   Structure: dam.
**   Test objective: groundwater flow analysis.
**
*NODE, NSET=Nall
       1, −3.00000e+01, −1.34110e−07,  0.00000e+00
       2, −3.00000e+01, −4.53062e−01,  0.00000e+00
       3, −2.45219e+01, −4.53062e−01,  0.00000e+00
...
*ELEMENT, TYPE=CPS8, ELSET=Eall
     1,      1,      2,      3,      4,      5,      6,      7,      8
     2,      4,      3,      9,     10,      7,     11,     12,     13
     3,     10,      9,     14,     15,     12,     16,     17,     18
...
*ELSET,ELSET=Earea1
1,
2,
...
*ELSET,ELSET=Earea2
161,
162,
...
*NSET,NSET=Nup
342,
345,
...
*NSET,NSET=Ndown
982,
985,
...
*MATERIAL,NAME=MAT1
*CONDUCTIVITY,TYPE=ORTHO
1.E−2,25.E−4,1.E−4
*MATERIAL,NAME=MAT2
*CONDUCTIVITY,TYPE=ORTHO
1.E−4,4.E−4,1.E−4
*SOLID SECTION,ELSET=Earea1,MATERIAL=MAT1
*SOLID SECTION,ELSET=Earea2,MATERIAL=MAT2
*INITIAL CONDITIONS,TYPE=TEMPERATURE
Nall,0.
**
*STEP
*HEAT TRANSFER,STEADY STATE
*BOUNDARY
Nup,11,11,8.5344
*BOUNDARY
Ndown,11,11,3.9624
*NODE PRINT,NSET=Nall
NT
*NODE FILE
NT
*EL FILE
HFL
*END STEP
```

Figure 21: Input deck of the dam problem

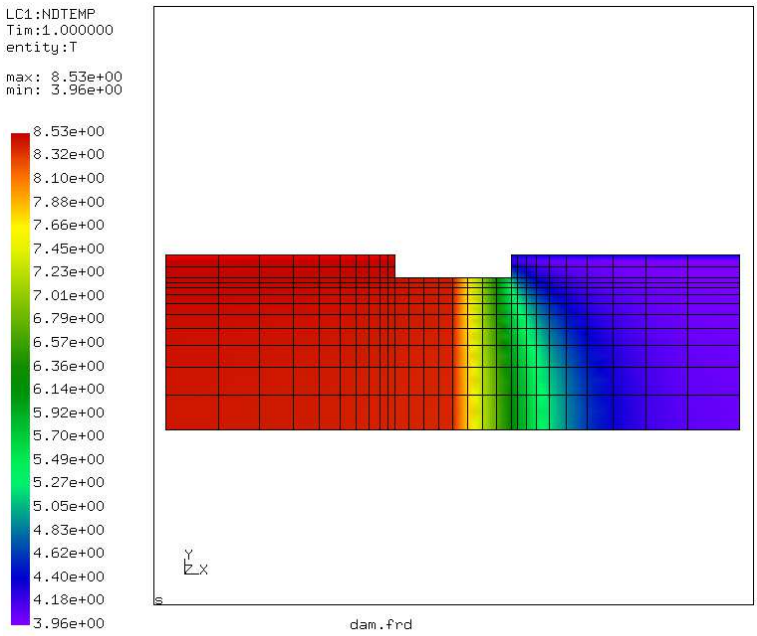


Figure 22: Total head

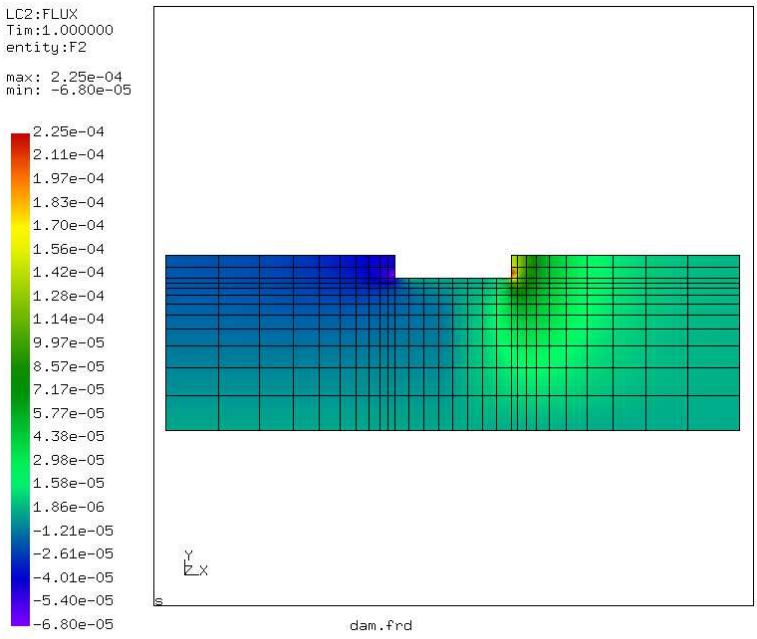


Figure 23: Discharge velocity in y-direction

the element sets for the two different kinds of soil are defined. The nodes on which the constant total head is to be applied are defined by *NSET cards. The permeability of the soil corresponds to the heat conduction coefficient in a thermal analysis. Notice that the permeability is defined to be orthotropic, using the *CONDUCTIVITY,TYPE=ORTHO card. The values beneath this card are the permeability in x, y and z-direction (SI units: m/s). The value for the z-direction is actually immaterial, since no gradient is expected in that direction. The *SOLID SECTION card is used to assign the materials to the appropriate soil regions. The *INITIAL CONDITIONS card is not really needed, since the calculation is stationary, however, CalculiX CrunchiX formally needs it in a heat transfer calculation.

Within the step a *HEAT TRANSFER, STEADY STATE calculation is selected without any additional time step information. This means that the defaults for the step length (1) and initial increment size (1) will be taken. With the *BOUNDARY cards the total head upstream and downstream is defined (11 is the temperature degree of freedom). Finally, the *NODE PRINT, *NODE FILE and *EL FILE cards are used to define the output: NT is the temperature, or, equivalently, the total head (Figure 22) , and HFL is the heat flux, or, equivalently, the groundwater flow velocity (y-component in Figure 23).

Since the permeability upstream is high, the total head gradient is small. The converse is true downstream. The flow velocity is especially important downstream. There it reaches values up to 2.25×10^{-4} m/s (the red spot in Figure 23), which corresponds to a hydraulic gradient of about 0.56, since the permeability in y-direction downstream is 4×10^{-4} m/s. This is smaller than 1, so no piping will occur. Notice that the velocity is naturally highest immediately next to the dam.

This example shows how seepage problems can be solved by using the heat transfer capabilities in CalculiX GraphiX. The same applies to any other phenomenon governed by a Laplace-type equation.

5.6 Capacitance of a cylindrical capacitor

In this section the capacitance of a cylindrical capacitor is calculated with inner radius 1 m, outer radius 2 m and length 10 m. The capacitor is filled with air, its permittivity is $\epsilon_0 = 8.8542 \times 10^{-12}$ C^2/Nm^2. An extract of the input deck, which is part of the test example suite, is shown below:

```
*NODE, NSET=Nall
...
*ELEMENT, TYPE=C3D20, ELSET=Eall
...
*NSET,NSET=Nin
1,
2,
...
*NSET,NSET=Nout
```

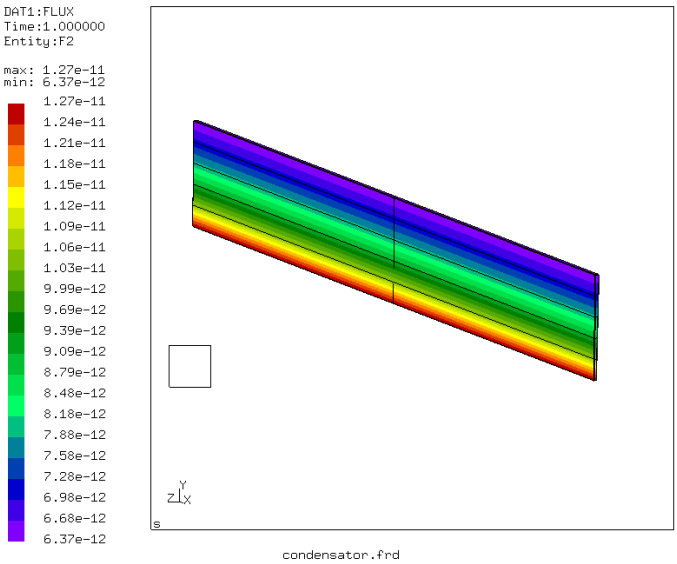


Figure 24: Heat flux in the capacitor's thermal analogy

```
57,
58,
...
*SURFACE,NAME=S1,TYPE=ELEMENT
6,S3
1,S3
*MATERIAL,NAME=EL
*CONDUCTIVITY
8.8541878176e-12
*SOLID SECTION,ELSET=Eall,MATERIAL=EL
*STEP
*HEAT TRANSFER,STEADY STATE
*BOUNDARY
Nin,11,11,2.
Nout,11,11,1.
*EL FILE
HFL
*FACE PRINT,SURFACE=S1
FLUX
*END STEP
```

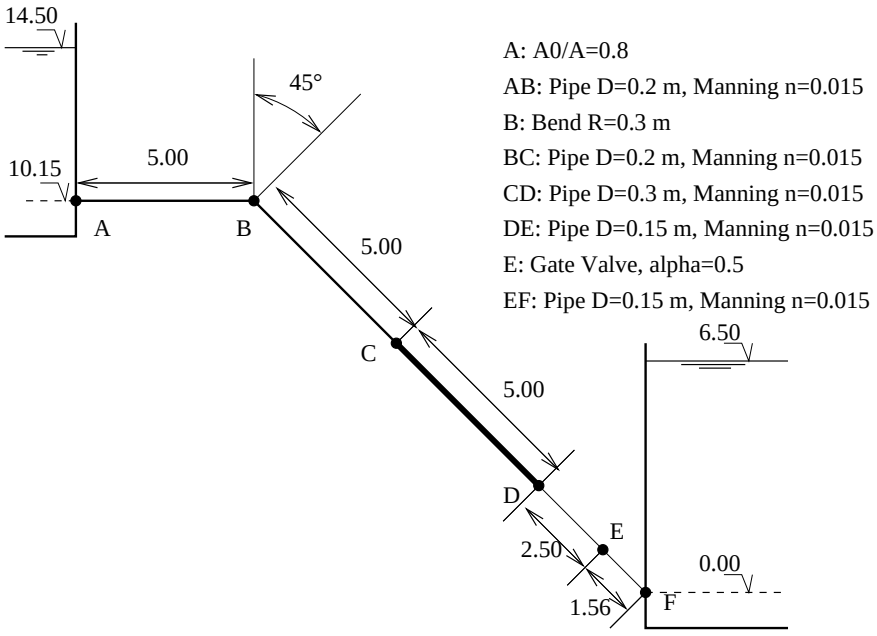


Figure 25: Geometry of the hydraulic network

As explained in Section 6.9.13 the capacitance can be calculated by determining the total heat flux through one of the capacitor's surfaces due to a unit temperature difference between the surfaces. The material in between the surfaces of the capacitor is assigned a conductivity equal to its permittivity. Here, only one degree of the capacitor has been modeled. In axial direction the mesh is very coarse, since no variation of the temperature is expected. Figure 24 shows that the heat flux at the inner radius is 1.27×10^{-11} W/m^2 . This corresponds to a total heat flow of 7.98^{-10} W. The analytical formula for the capacitor yields $2\pi\epsilon_0/\ln(2) = 8.0261^{-10}$ C/V.

The total flux through the inner surface S1 is also stored in the .dat file because of the *FACE PRINT keyword card in the input deck. It amounts to -2.217×10^{-12} W. This value is negative, because the flux is entering the space in between the capacitor's surfaces. Since only one degree was modeled, this value has to be multiplied by 360 and yields the same value as above.

5.7 Hydraulic pipe system

In CalculiX it is possible to perform steady-state hydraulic and aerodynamic network calculations, either as stand-alone applications, or together with mechanical and/or thermal calculations of the adjacent structures. Here, a stand-alone hydraulic network discussed in [10] is analyzed. The input deck pipe.f can be found in the test suite.

The geometry of the network is shown in Figure 25. It is a linear network consisting of:

- an upstream reservoir with surface level at 14.5 m
- an entrance with a contraction of 0.8
- a pipe with a length of 5 m and a diameter of 0.2 m
- a bend of 45 ^{o} and a radius of 0.3 m
- a pipe with a length of 5 m and a diameter of 0.2 m
- a pipe with a length of 5 m and a diameter of 0.3 m
- a pipe with a length of 2.5 m and a diameter of 0.15 m
- a gate valve in E with $\alpha = 0.5$
- a pipe with a length of 1.56 m and a diameter of 0.15 m
- an exit in a reservoir with surface level at 6.5 m

All pipes are characterized by a Manning friction coefficient n=0.015. The input deck looks like:

```
**
**   Structure: pipe connecting two reservoirs.
**   Test objective: hydraulic network.
**
*NODE,NSET=NALL
2,0.,0.,14.5
3,0.,0.,14.5
4,0.,0.,12.325
...
26,14.9419,0.,6.5
*ELEMENT,TYPE=D,ELSET=EALL
1,0,2,3
2,3,4,5
...
13,25,26,0
*MATERIAL,NAME=WATER
*DENSITY
1000.
*FLUID CONSTANTS
4217.,1750.E-6,273.
*ELSET,ELSET=E1
2
*ELSET,ELSET=E2
```

```
3,5
*ELSET,ELSET=E3
4
*ELSET,ELSET=E4
6
*ELSET,ELSET=E5
7
*ELSET,ELSET=E6
8
*ELSET,ELSET=E7
9,11
*ELSET,ELSET=E8
10
*ELSET,ELSET=E9
12
*ELSET,ELSET=E10
1,13
*FLUID SECTION,ELSET=E1,TYPE=PIPE ENTRANCE,MATERIAL=WATER
0.031416,0.025133
*FLUID SECTION,ELSET=E2,TYPE=PIPE MANNING,MATERIAL=WATER
0.031416,0.05,0.015
*FLUID SECTION,ELSET=E3,TYPE=PIPE BEND,MATERIAL=WATER
0.031416,1.5,45.,0.4
*FLUID SECTION,ELSET=E4,TYPE=PIPE ENLARGEMENT,MATERIAL=WATER
0.031416,0.070686
*FLUID SECTION,ELSET=E5,TYPE=PIPE MANNING,MATERIAL=WATER
0.070686,0.075,0.015
*FLUID SECTION,ELSET=E6,TYPE=PIPE CONTRACTION,MATERIAL=WATER
0.070686,0.017671
*FLUID SECTION,ELSET=E7,TYPE=PIPE MANNING,MATERIAL=WATER
0.017671,0.0375,0.015
*FLUID SECTION,ELSET=E8,TYPE=PIPE GATE VALVE,MATERIAL=WATER
0.017671,0.5
*FLUID SECTION,ELSET=E9,TYPE=PIPE ENLARGEMENT,MATERIAL=WATER
0.017671,1.E6
*FLUID SECTION,ELSET=E10,TYPE=PIPE INOUT,MATERIAL=WATER
*BOUNDARY
3,2,2,1.E5
25,2,2,1.E5
*STEP
*HEAT TRANSFER,STEADY STATE
*DLOAD
EALL,GRAV,9.81,0.,0.,-1.
*NODE PRINT,NSET=NALL
U
*END STEP
```

In CalculiX linear networks are modeled by means of 3-node network elements (D-type elements). In the corner nodes of the element the temperature and the pressure are unknown. They are assigned to the degrees of freedom 0 and 2, respectively. In the midside node the mass flux is unknown and is assigned to degree of freedom 1. The properties of the network elements are defined by the keyword *FLUID SECTION. They are treated extensively in Section 6.4 (gases), 6.5 (liquid pipes) and 6.6 (liquid channels). For the network at stake we need:

- a dummy network entrance element expressing that liquid is entering the network (element 1). It is characterized by a node number 0 as first node
- a network element of type PIPE ENTRANCE at location A (element 2). This element also takes the water depth into account. Notice that there is no special reservoir element. Differences in water level can be taken into account in any element type by assigning the appropriate coordinates to the corner nodes of the element.
- a network element of type PIPE MANNING for the pipe between location A and B (element 3)
- a network element of type PIPE BEND for the bend at location B (element 4)
- a network element of type PIPE MANNING for the pipe between location B and C (element 5)
- a network element of type PIPE ENLARGEMENT for the increase of diameter at location C (element 6)
- a network element of type PIPE MANNING for the pipe between location C and D (element 7)
- a network element of type PIPE CONTRACTION to model the decrease in diameter at location D (element 8)
- a network element of type PIPE MANNING for the pipe between location D and E (element 9)
- a network element of type PIPE GATE VALVE for the valve at location E (element 10)
- a network element of type PIPE MANNING for the pipe between location E and F (element 11)
- a network element of type PIPE ENLARGEMENT for the exit in the reservoir (element 12). Indeed, there is no special reservoir entrance element. A reservoir entrance has to be modeled by a large diameter increase.
- a dummy network exit element expressing that liquid is leaving the network (element 13)

In the input deck, all these elements are defined as D-type elements, their nodes have the correct coordinates and by means of *FLUID SECTION cards each element is properly described. Notice that the dummy network entrance and exit elements are characterized by typeless *FLUID SECTION cards.

For a hydraulic network the material properties reduce to the density (on the *DENSITY card), the specific heat and the dynamic viscosity (both on the *FLUID SECTION card). The specific heat is only needed if heat transfer is being modeled. Here, this is not the case. The dynamic viscosity of water is 1750×10^{-6}N s/m^2 [34]. The boundary conditions reduce to the atmospheric pressure in node 3 and 25, both at the liquid surface of the reservoir. Remember that the pressure has the degree of freedom 2 in the corner nodes of the network elements.

Networks are only active in *COUPLED TEMPERATURE-DISPLACEMENT or *HEAT TRANSFER procedures. Here, we do not take the structure into account, so a heat transfer analysis will do. Finally, the gravity loading has to be specified, this is indeed essential for hydraulic networks. Regarding the nodal output, remember that NT requests degree of freedom 0, whereas U requests degrees of freedom 1 to 3. Since we are interested in the mass flux (DOF 1 in the middle nodes) and the pressure (DOF 2 in the corner nodes), U is selected underneath the *NODE PRINT line. Officially, U are displacements, and that's the way they are labeled in the .dat file.

The results in the .dat file look as follows:

```
displacements (vx,vy,vz) for set NALL and time   1.

     2  8.9592E+01  0.0000E+00  0.0000E+00
     3  0.0000E+00  1.0000E+05  0.0000E+00
     4  8.9592E+01  0.0000E+00  0.0000E+00
     5  0.0000E+00  1.3386E+05  0.0000E+00
     6  8.9592E+01  0.0000E+00  0.0000E+00
     7  0.0000E+00  1.2900E+05  0.0000E+00
     8  8.9592E+01  0.0000E+00  0.0000E+00
     9  0.0000E+00  1.2859E+05  0.0000E+00
    10  8.9592E+01  0.0000E+00  0.0000E+00
    11  0.0000E+00  1.5841E+05  0.0000E+00
    12  8.9592E+01  0.0000E+00  0.0000E+00
    13  0.0000E+00  1.6040E+05  0.0000E+00
    14  8.9592E+01  0.0000E+00  0.0000E+00
    15  0.0000E+00  1.9453E+05  0.0000E+00
    16  8.9592E+01  0.0000E+00  0.0000E+00
    17  0.0000E+00  1.7755E+05  0.0000E+00
    18  8.9592E+01  0.0000E+00  0.0000E+00
    19  0.0000E+00  1.8361E+05  0.0000E+00
    20  8.9592E+01  0.0000E+00  0.0000E+00
    21  0.0000E+00  1.5794E+05  0.0000E+00
```

```
 22  8.9592E+01  0.0000E+00  0.0000E+00
 23  0.0000E+00  1.6172E+05  0.0000E+00
 24  8.9592E+01  0.0000E+00  0.0000E+00
 25  0.0000E+00  1.0000E+05  0.0000E+00
 26  8.9592E+01  0.0000E+00  0.0000E+00
```

The mass flux in the pipe (first DOF in the midside nodes, column 1) is constant and takes the value 89.592 kg/s. This agrees well with the result in [10] of 89.4 l/s. Since not all node and element definitions are listed it is useful for the interpretation of the output to know that location A corresponds to node 5, location B to nodes 7-9, location C to nodes 11-13, location D to nodes 15-17, location E to nodes 19-21 and location F to node 23. The second column in the result file is the pressure. It shows that the bend, the valve and the contraction lead to a pressure decrease, whereas the enlargement leads to a pressure increase (the velocity drops).

If the structural side of the network (e.g. pipe walls) is modeled too, the fluid pressure can be mapped automatically onto the structural element faces. This is done by labels of type PxNP in the *DLOAD card.

5.8 Lid-driven cavity

The lid-driven cavity is a well-known benchmark problem for viscous incompressible fluid flow [79]. The geometry at stake is shown in Figure 26. We are dealing with a square cavity consisting of three rigid walls with no-slip conditions and a lid moving with a tangential unit velocity. We are interested in the velocity and pressure distribution for a Reynolds number of 400.

The input deck looks like (this deck is also available in the cfd test suite as file lid400.inp):

```
**
** Structure: lid-driven cavity
** Test objective: incompressible, viscous, laminar, 3D fluid
**
*NODE, NSET=Nall
       1,5.000000000000e-01,5.000000000000e-01,0.0
...
*ELEMENT, TYPE=F3D8, ELSET=Eall
     1,     1,     2,     3,     4,     5,     6,     7,     8
...
*SURFACE, NAME=SOLIDSURFACE
40, S2
...
*MATERIAL,NAME=WATER
*DENSITY
1.
```

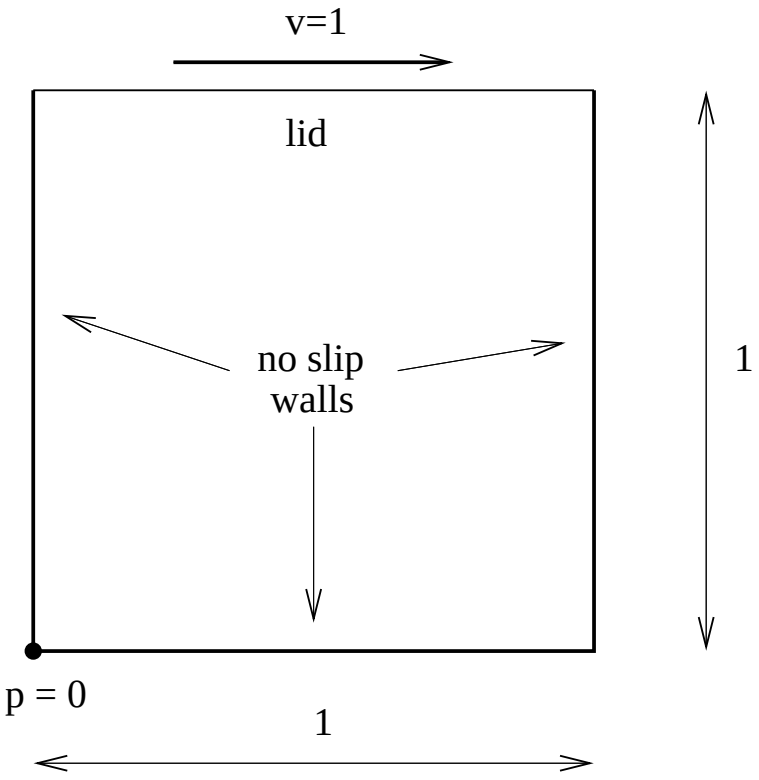


Figure 26: Geometry of the lid-driven cavity

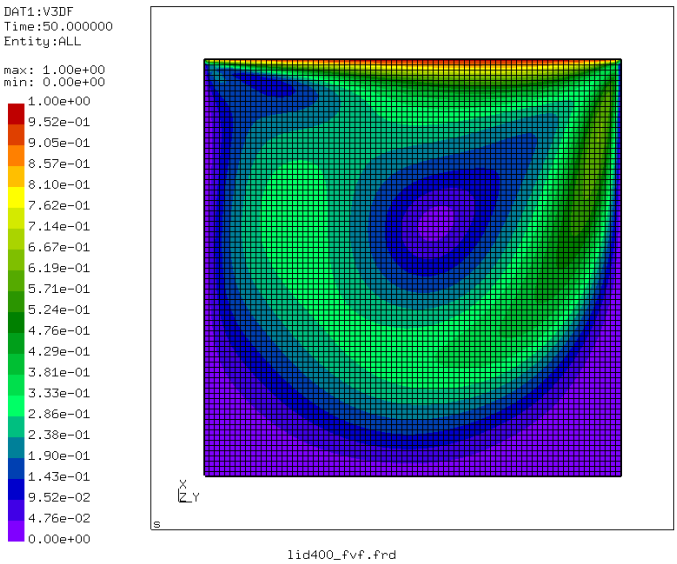


Figure 27: Mesh of the lid-driven cavity

```
*FLUID CONSTANTS
1.,.25E-2,293.
*SOLID SECTION,ELSET=Eall,MATERIAL=WATER
*INITIAL CONDITIONS,TYPE=FLUID VELOCITY
Nall,1,0.
Nall,2,0.
Nall,3,0.
*INITIAL CONDITIONS,TYPE=PRESSURE
Nall,1.
**
*STEP,INCF=5000
*STATIC
*BOUNDARYF
** BOUNDARYF based on fixz
1, S3, 3,, 0.000000
...
** BOUNDARYF based on in
1601, S1, 1,, 0.000000
...
** BOUNDARYF based on in
1601, S1, 2,, 1.000000
...
** BOUNDARYF based on in
```

```
1601, S1, 3,, 0.000000
...
** BOUNDARYF based on wall
40, S2, 1,, 0.000000
...
** BOUNDARYF based on wall
40, S2, 2,, 0.000000
...
** BOUNDARYF based on wall
40, S2, 3,, 0.000000
...
*BOUNDARYF
1600, S3, 8,8, 1.000000
*NODE FILE,FREQUENCYF=5000
VF,PSF
*END STEP
```

Although the problem is essentially 2-dimensional it was modeled as a 3-dimensional problem with unit thickness since 2-dimensional fluid capabilities are not available in CalculiX. The mesh (2D projection) is shown in Figure 27. It consists of 8-node brick elements. There is one element layer across the thickness. This is sufficient, since the results do not vary in thickness direction. The input deck starts with the coordinates of the nodes and the topology of the elements. The element type for fluid volumetric elements is the same as for structural elements with the C replaced by F (fluid): F3D6. The faces belonging to solid surfaces are listed next. A face is characterized by an element number and an internal face number. Solid surfaces are surfaces at which the fluid adheres, i.e. in the presence of viscosity the velocity vector adjacent to a solid surface is the same as the velocity of the surface itself. All solid surfaces must be collected into a SURFACE definition with the name SOLIDSURFACE (no upper case required, though).

The material definition consists of the density, the heat capacity and the dynamic viscosity. The density is set to 1. The heat capacity and the dynamic viscosity are entered underneath the *FLUID CONSTANTS keyword. The heat capacity is not needed since the calculation is steady state, so its value here is irrelevant. The value of the dynamic viscosity was chosen such that the Reynolds number is 400. The Reynolds number is defined as velocity times length divided by the kinematic viscosity. The velocity of the lid is 1, its length is 1 and since the density is 1 the kinematic and dynamic viscosity coincide. Consequently, the kinematic viscosity takes the value 1/400. The material is assigned to the elements by means of the *SOLID SECTION card.

The unknowns of the problem are the velocity and static pressure. No thermal boundary conditions are provided, so the temperature is irrelevant. All initial values for the velocity and pressure are set by means of the *INITIAL CONDITIONS,TYPE=FLUID VELOCITY and *INITIAL CONDITIONS,TYPE=PRESSURE cards. Notice that for the velocity the initial conditions have to be specified for

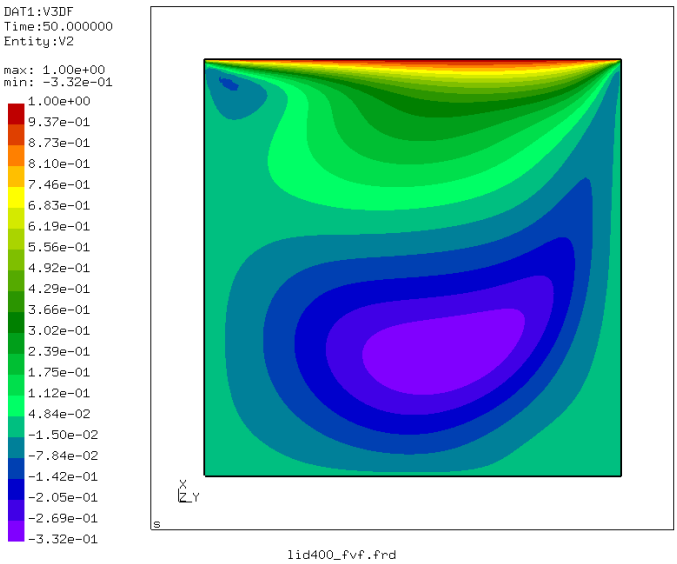


Figure 28: y-component of the velocity in the lid-driven cavity

each degree of freedom separately.

The step is as usual started with the *STEP keyword. The maximum number of increments, however, is for fluid calculations governed by the parameter INCF. For steady state calculations the keyword *STATIC is to be used. If there are no time increment values beneath this line the increment size is automatically chosen such that the procedure is stable. The boundary conditions for fluid calculations are defined on the faces and are prescribed using the *BOUNDARYF card. Recall that non-homogeneous (i.e. nonzero) boundary conditions have to be defined within a step, homogeneous ones may be defined before or within the step. Here, all boundary conditions have been defined within the step. They include zero velocity at the fixed walls, a velocity of 1 in the y-direction on the lid, and zero velocity in z-direction on the side walls. The pressure has been set to 1 on face 3 of element 1600. In CFD pressure boundary conditions can only be set on faces for which not all velocity components are prescribed. Consequently, in the present example, the pressure could not have been set on faces belonging to the walls and the lid.

The step ends with a nodal print request for the velocity VF and the static pressure PSF. The printing frequency is defined to be 5000 by means of the FREQUENCYF parameter. This means, that results will be stored every 5000 increments.

The velocity distribution in y-direction (i.e. the direction tangential to the lid) is shown in Figure 28. The smallest value (-0.33) and its location agree very well with the results in [79]. Figure 29 shows a vector plot of the velocity. Near

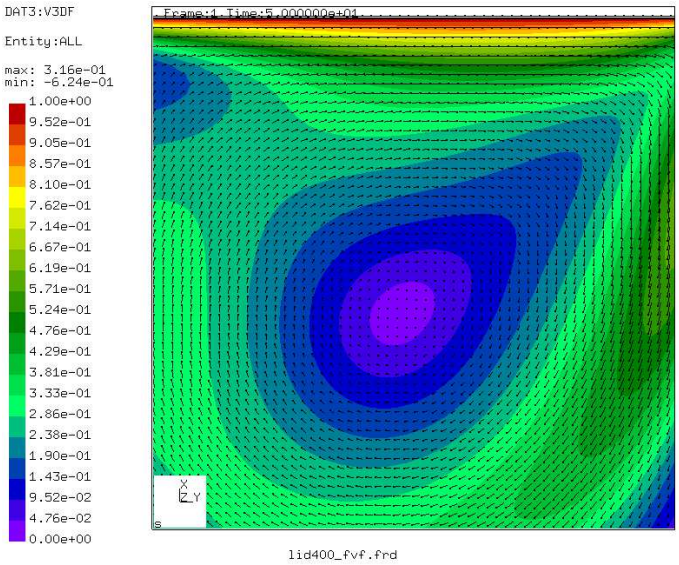


Figure 29: Velocity distribution in the lid-driven cavity (excerpt)

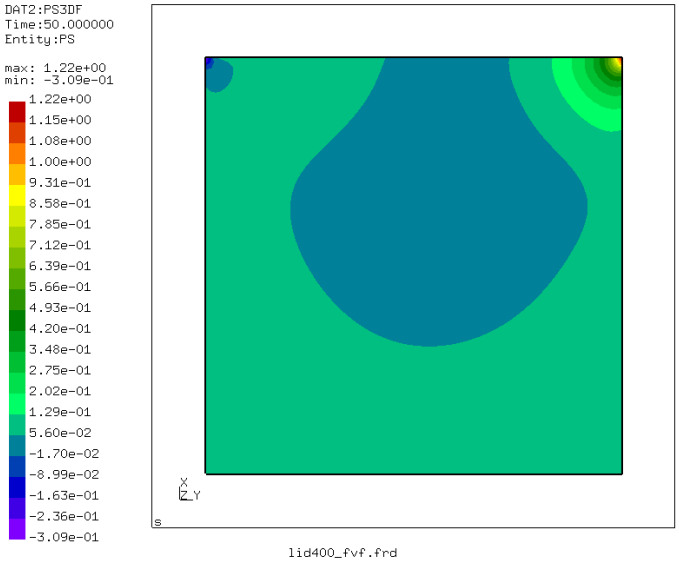


Figure 30: Pressure distribution in the lid-driven cavity

the lid there is a large gradient, in the lower left and lower right corner are dead zones. The pressure plot (Figure 30) reveals a low pressure zone in the center of the major vortex and in the left upper corner. The right upper corner is a stagnation point for the y-component of the velocity and is characterized by a significant pressure built-up.

5.9 Transient laminar incompressible Couette problem

Another well-known problem is the incompressible laminar flow between two parallel plates. At time zero both plates are at rest, whereas at positive times one of the plates is moved parallel to the other plate with a velocity of 1. The analytical solution can be found in [62] in the form of a series expansion containing the complementary error function erfc. In the steady state regime the velocity profile is linear across the space in between the plates. The velocity profiles at different times are shown in Figure 31 and compared with the analytical solution for a unity distance between the plates and a kinematic viscosity $\nu = 1$. The input deck for the CalculiX results can be found in the test suite (couette1.inp). A time increment of 0.00012376 was chosen to obtain good results. It is yet unclear, how to calculate the increment needed to obtain correct predictions. The only feasible procedure right now is to try increasingly small increments unless the results do not change any more. The figure shows good agreement between the numerical and analytical values, indicating that the time integration in the CFD-implementation in CalculiX is correct. The small deviations at small times are due to the rather coarse mesh.

5.10 Stationary laminar inviscid compressible airfoil flow

Note: compressible CFD-calculations have been deactivated in version 2.7 due to unsatisfactory results. A new approach is being pursued.

In [59] the results of CFD-calculations for several airfoils are reported. Here, the computations for $M_\infty = 1.2$ (Mach number at infinity) and $\alpha = 7.$ (angle of attack) are reported. The input deck for this calculation can be found in the fluid examples test suite (agard05.inp).

To explain the differences in the input deck between incompressible and compressible flow the crucial section from the compressible input deck is reproduced below.

```
*EQUATION
2
3,2,-0.99030509E+00,3,1,-0.13890940E+00
2
3756,2,-0.99030509E+00,3756,1,-0.13890940E+00
...
*MATERIAL,NAME=AIR
*CONDUCTIVITY
0.
```

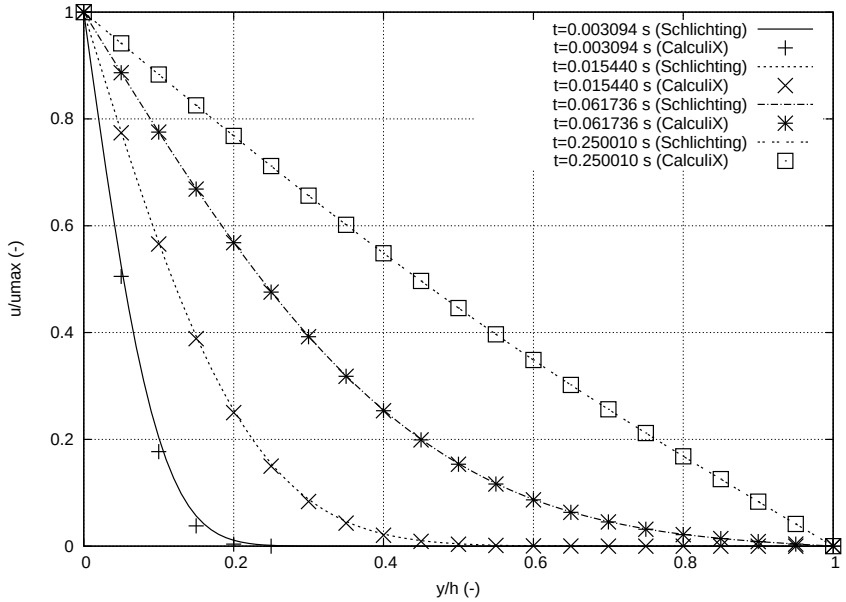


Figure 31: Velocity across the space in between the plates for different times

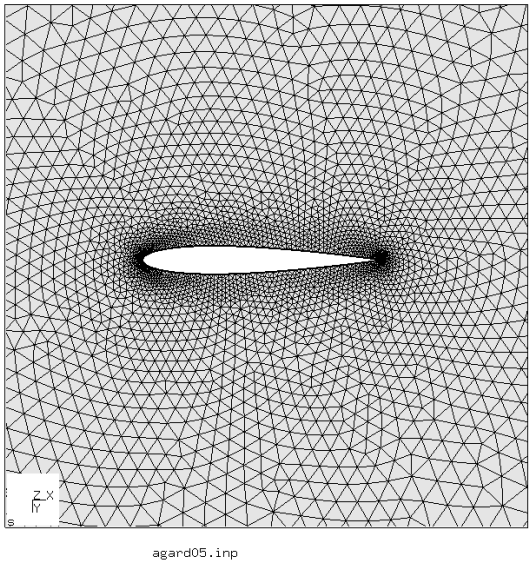


Figure 32: Mesh for the naca012 airfoil flow

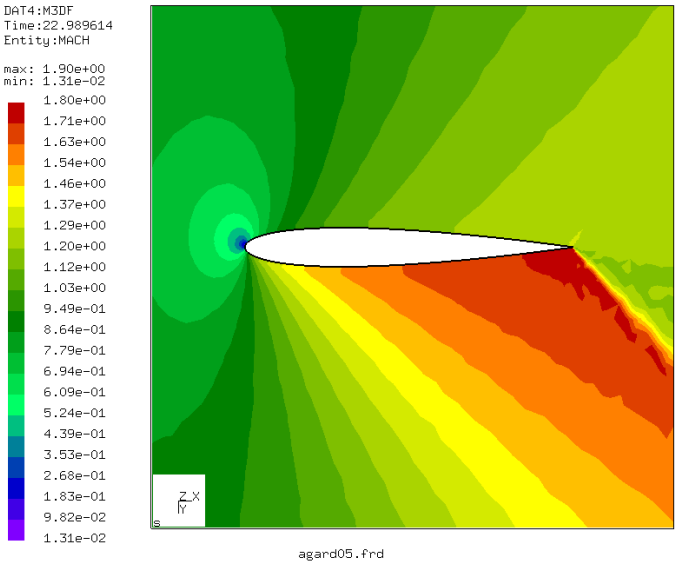


Figure 33: Mach number in the naca012 airfoil flow

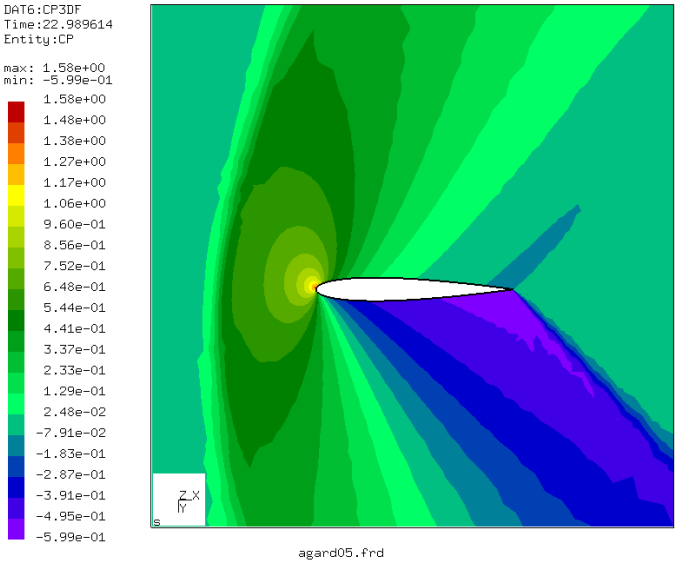


Figure 34: Pressure coefficient in the naca012 airfoil flow

```
*FLUID CONSTANTS
1.,1.d-20,293.
*SPECIFIC GAS CONSTANT
0.285714286d0
*SOLID SECTION,ELSET=Eall,MATERIAL=AIR
*PHYSICAL CONSTANTS,ABSOLUTE ZERO=0.
*INITIAL CONDITIONS,TYPE=FLUID VELOCITY
Nall,1,0.99254615
Nall,2,0.12186934
Nall,3,0.d0
*INITIAL CONDITIONS,TYPE=PRESSURE
Nall,0.49603175
*INITIAL CONDITIONS,TYPE=TEMPERATURE
Nall,1.73611111
*VALUES AT INFINITY
1.73611111,1.,0.49603175,1.,1.
**
*STEP,INCF=40000,SHOCK SMOOTHING=0.1
*STATIC,EXPLICIT
1.,1.
*BOUNDARY
BOU1,11,11,1.73611111
BOU1,1,1,0.99254615
BOU1,2,2,0.12186934
BOU1,8,8,0.49603175
Nall,3,3,0.
*NODE FILE,FREQUENCYF=40000
V,PS,CP,TS,TT,MACH
*END STEP
```

Since for compressible flow the temperature, velocity and pressure are linked through the ideal gas equation, the definition of the thermal conductivity and specific heat is mandatory. Inviscid flow was triggered by the definition of a very low viscosity AND slip boundary conditions at the airfoil surface through equations. The specific gas constant is defined with the appopriate keyword. It only depends on the kind of gas and not on the temperature. The physical constants card is used to define absolute zero for the temperature scale. This information is needed since the temperature in the gas equation must be specified in Kelvin. Initial conditions must be specified for the velocity, pressure and temperature. Careful selection of these values can shorten the computational time. The values at infinity (defined with the *VALUES AT INFINITY card) are used to calculate the pressure coefficient. In viscous calculations they are used for the computation of the friction coefficient too. The smoothing parameter on the *STEP card is used to define shock smoothing and will be discussed in the next paragraph. Finally, compressible calculations are performed explicitly. Therefore, the EXPLICIT parameter on the *STATIC or *DYNAMIC keyword

is mandatory. It is the EXPLICIT parameter which tells CalculiX whether the flow is compressible or incompressible. With the EXPLICIT parameter the flow is assumed to be compressible, else it is assumed to be incompressible. The use of the *STATIC keyword tells CalculiX that the calculation is stationary. Instationary calculations are triggered with the *DYNAMIC keyword. In reality, all CFD-calculations in CalculiX are instationary. The *STATIC keyword, however, forces the calculations to be pursued until steady state is reached (so the time used is virtual). Dynamic calculations stop as soon as the final time is reached (the time is real).

In compressible calculations shock smoothing is frequently needed in order to avoid divergence. Shock smoothing, however, can change the solution. Therefore, the shock smoothing coefficient, which can take values between 0. and 2., should be chosen as small as possible. For the agard05 example a value of 0.1 was needed. In general, additional viscosity will reduced the shock smoothing needed to avoid divergence. There is a second effect of the shock smoothing coefficient: there is no clear steady state convergence any more. In order to understand this some additional information about the way CFD-calculations in CalculiX are performed. The initial increment size which is specified by the user underneath the *STATIC or *DYNAMIC card is a mechanical increment size. For each mechanical increment an instationary CFD-calculation is performed subject to the actual loads (up to steady state for a *STATIC calculation). For this CFD-calculations subincrements are used, the size of which depends on the physical characteristics of the flow (viscosity, heat conductivity etc.). They are determined such that stability is assured (or at least very likely). In CalculiX, steady state convergence is detected as soon as the change in the conservative variables ($\rho, \rho u, \rho v$ etc.) from subincrement to subincrement does not exceed $1.^{-8}$ times the actual values of these variables. In calculations with a nonzero shock smoothing coefficient the change in variables at first decreases down to a certain level about which it oscillates erraticaly. In that case, steady state is detected as soon as the tangent of a linear regression curve through the last half of the change in variables values drops below a given number. The change in the conservative variables is stored in a file with the name jobname.cvg. The user may force convergence by limiting the number of subincrements with the INCF parameter on the *STEP card. As soon as INCF subincrements are calculated the CFD-calculation is assumed to be finished and the next mechanical increment is started.

Figure 32 shows the mesh used for the agard05 calculation. It consists of linear wedge elements. In CalculiX, only linear elements (tetrahedra, hexahedra or wedges) are allowed for CFD-calculations. It is finer along the airfoil (but not as fine as needed to capture the boundary layer in viscous calculations). Figures 33 and 34 shows the Mach number and the pressure coefficient, respectively. The maximum Mach number in [59] is about 1.78, the maximum pressure coefficient is about -0.55. This agrees well with the present results. Increasing the shock smoothing coefficient leads to smoothing fringe plots, however, the actual values become worse.

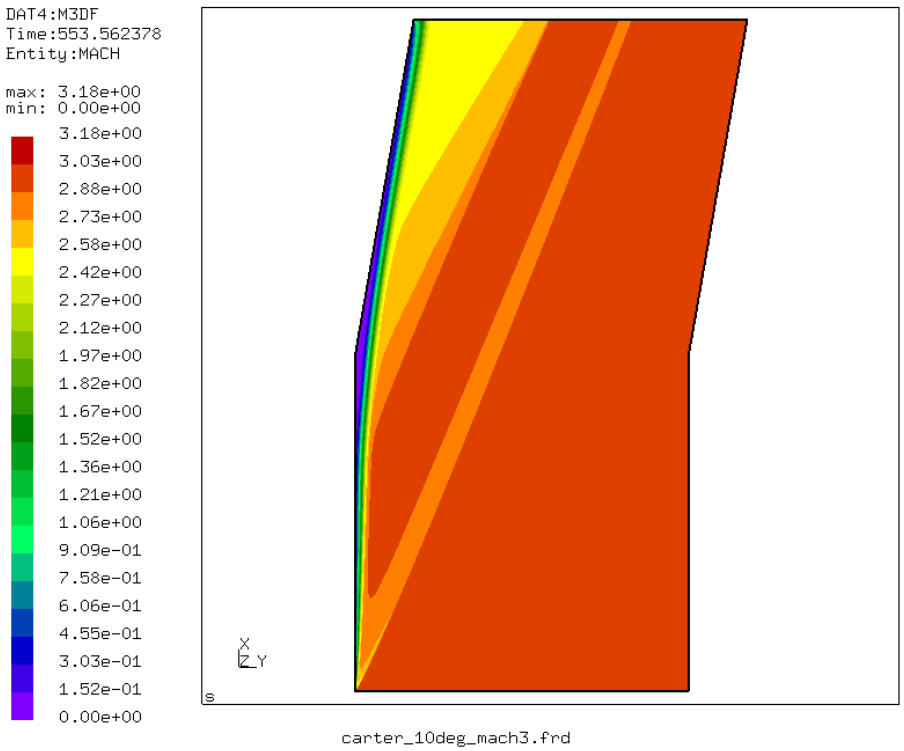


Figure 35: Mach number for the Carter problem

5.11 Laminar viscous compressible compression corner flow

Note: compressible CFD-calculations have been deactivated in version 2.7 due to unsatisfactory results. A new approach is being pursued.

This benchmark example is described in [15]. The input deck for the CalculiX computation is called carter_10deg_mach3.inp and can be found in the fluid test example suite. The flow is entering at Mach 3 parallel to a plate of length 16.8 after which a corner of 10° arises. The Reynolds number based on a unit length is 1000., which yields for a unit velocity a dynamic viscosity coefficient $\mu = 10^{-3}$. No units are specified: the user can choose appropriate consistent units. Choosing $c_p = 1$ and $\kappa = 1.4$ leads to a specific gas constant $r = 0.286$. The selected Mach number leads to an inlet temperature of $T = 0.778$. The ideal gas law yields a static inlet pressure of $p = 0.0794$ (assuming an unit inlet density). The wall is assumed to be isothermal at a total temperature of $T_t = 0.778$. Finally, the assumed Prandl number (Pr=$\mu c_p/\lambda$) of 0.72 leads to a conduction coefficient of 0.00139.

A very fine mesh with about 425,000 nodes was generated, gradually finer

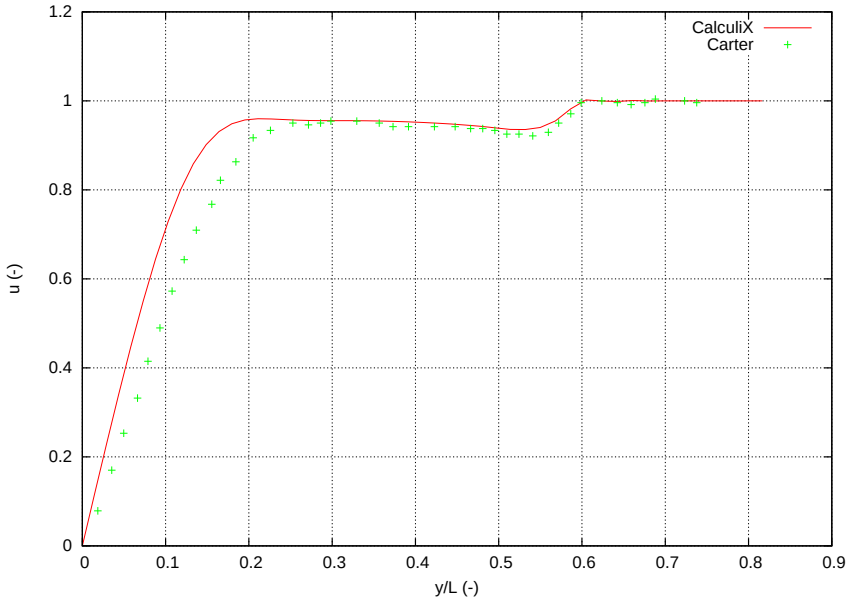


Figure 36: velocity profile across the flow for the Carter problem

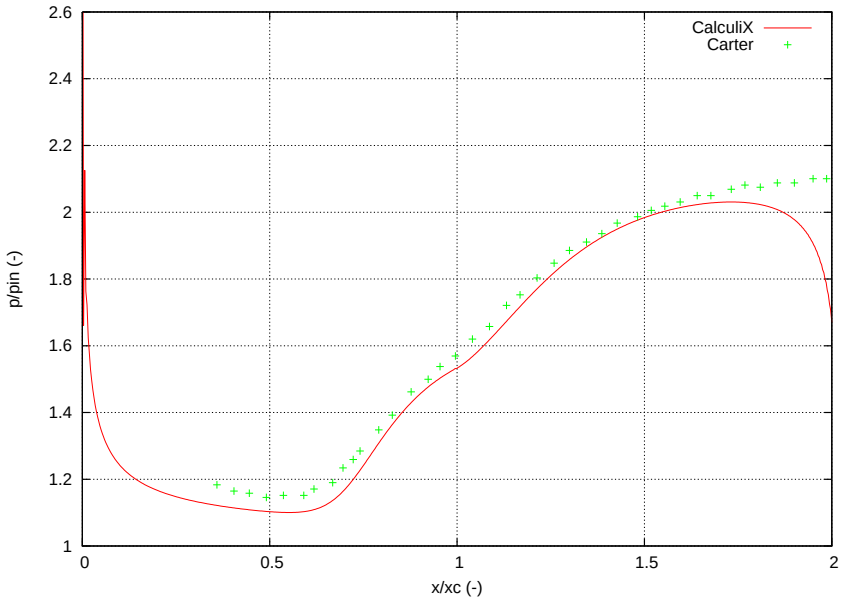


Figure 37: Static pressure at the wall for the Carter problem

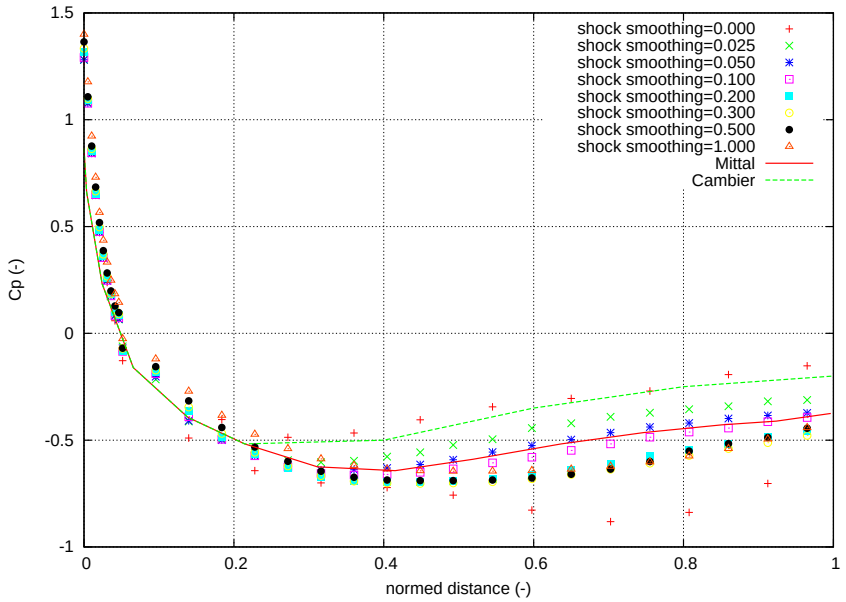


Figure 38: Pressure coefficient for laminar viscous flow about a naca012 airfoil

towards the wall ($y^+ = 1.28$ for the closest node near the wall at L=1 from the inlet). The Mach number is shown in Figure 35. The shock wave emanating from the front of the plate and the separation and reattachment compression fan at the kink in the plate are cleary visible. One also observes the thickening of the boundary layer near the kink leading to a recirculation zone. Figure 36 shows the velocity component parallel to the inlet plate orientation across a line perpendicular to a plate at unit length from the entrance. One notices that the boundary layer in the CalculiX calculation is smaller than in the Carter solution. This is caused by the temperature-independent viscosity. Applying the Sutherland viscosity law leads to the same boundary layer thickness as in the reference. In CalculiX, no additional shock smoothing was necessary. Figure 37 plots the static pressure at the wall relative to the inlet pressure versus a normalized plate length. The reference length for the normalization was the length of the plate between inlet and kink (16.8 unit lengths). So the normalized length of 1 corresponds to the kink. There is a good agreement between the CalculiX and the Carter results, apart from the outlet zone, where the outlet boundary conditions influence the CalculiX results.

5.12 Laminar viscous compressible airfoil flow

Note: compressible CFD-calculations have been deactivated in version 2.7 due to unsatisfactory results. A new approach is being pursued.

A further example is the laminar viscous compressible flow about a naca012

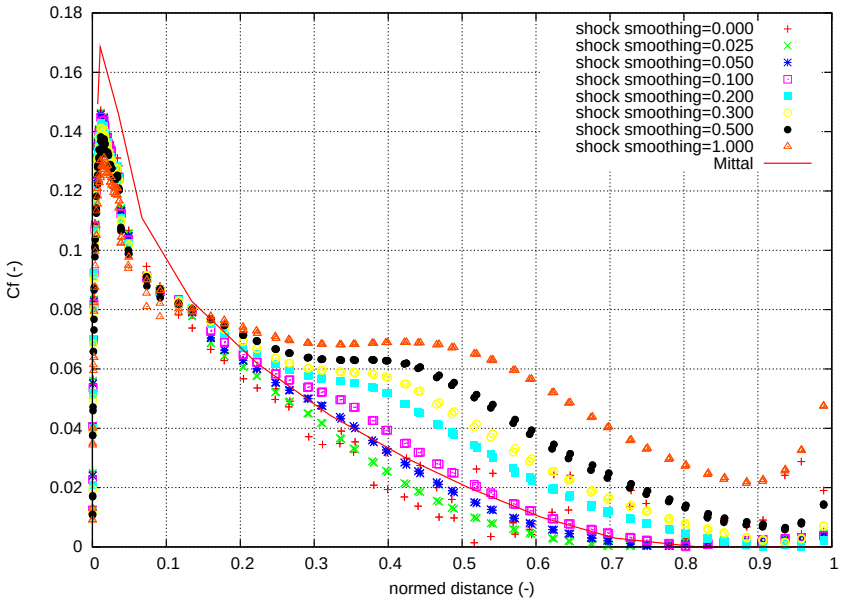


Figure 39: Friction coefficient for laminar viscous flow about a naca012 airfoil

airfoil. Results for this problem were reported by [54]. The entrance Mach number is 0.85, the Reynolds number is 2000. Of interest is the steady state solution. In CalculiX this is obtained by performing a transient CFD-calculation up to steady state. The input deck for this example is called naca012_visc_mach0.85.inp and can be found amoung the CFD test examples. Basing the Reynolds number on the unity chord length of the airfoil, an entrance unity velocity and a entrance unity density leads to a dynamic viscosity of $\mu = 5 \times 10^{-4}$. Taking $c_p = 1$ and $\kappa = 1.4$ leads to a specific gas constant $r = 0.2857$ (all in consistent units). Use of gthe entrance Mach number determines the entrance static temperature to be $T_s = 3.46$. Finally, the ideal gas law leads to a entrance static pressure of $p_s = 0.989$. Taking the Prandl number to be one determines the heat conductivity $\lambda = 5^{-4}$. The surface of the airfoil is assumed to be adiabatic.

The results for the pressure and the friction coefficient at the surface of the airfoil are shown in Figures 38 and 39, respecively, as a function of the shock smoothing coefficient. The pressure coefficient is defined by $c_p = (p - p_\infty)/(0.5\rho_\infty v_\infty^2)$, where p is the local static pressure, p_∞, ρ_∞ and v_∞ are the static pressure, density and velocity at the entrance, respectively. From Figure 38 it is clear that a reduction of the shock smoothing coefficient improves the results. For a zero shock smoothing coefficient, however, the results oscillate and do not make sense any more. Taking into account that the reference results do not totally agree either, a shock smoothing coefficient of 0.025, which is the smallest smoothing coefficient yielding non-oscillating values, leads to the

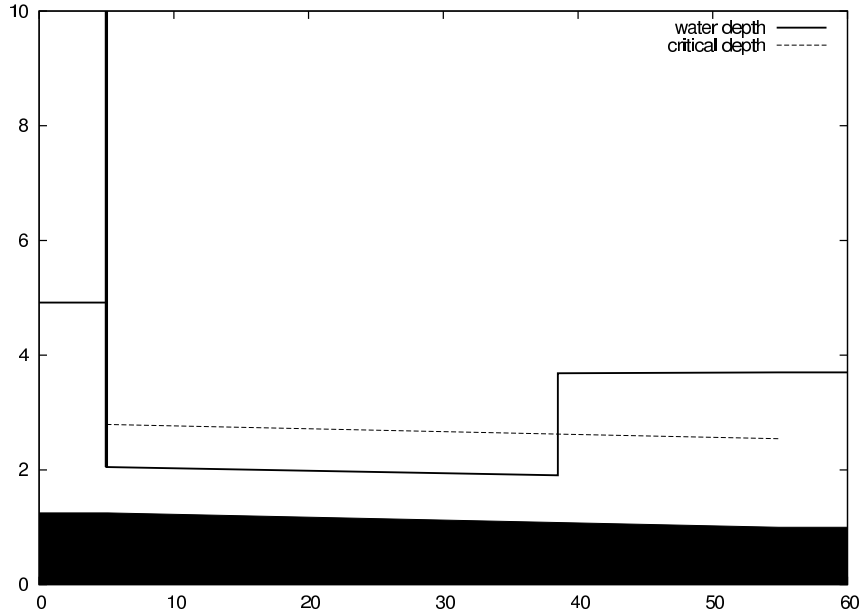


Figure 40: Water depth in a channel with hydraulic jump

best results. The friction coefficient is defined by $\tau_w/(0.5\rho_\infty v_\infty^2)$, where τ_w is the local shear stress. Here too, a too large shock smoothing coefficient clearly leads to wrong results. A value of 0.05 best agrees with the results by Mittal, however, in the light of the c_p-results from the literature a value of 0.025 might be good as well. The c_f-peak at the front of the airfoil is not very well hit: the literature result is 0.17, the CalculiX peak reaches only up to 0.15. While decreasing the shock smoothing coefficient increases the peak, a too coarse mesh density at that location may also play a role. The general advice is to use as little shock smoothing as possible.

5.13 Channel with hydraulic jump

That open channel flow can be modeled as a one-dimensional network is maybe not so well known. The governing equation is the Bresse equation (cf. Section 6.9.18) and the available fluid section types are listed in Section 6.6.

The input deck for the present example is shown below.

```
**
**   Structure: channel connecting two reservoirs.
**   Test objective: steep slope, frontwater - jump -
**                   backwater curve
**
*NODE,NSET=NALL
```

```
1,0.,0.,0.
2,1.,0.,0.
3,2.,0.,0.
4,3.,0.,0.
5,4.,0.,0.
6,5.,0.,0.
7,6.,0.,0.
8,7.,0.,0.
9,8.,0.,0.
10,9.,0.,0.
11,10.,0.,0.
*ELEMENT,TYPE=D,ELSET=EALL
1,0,1,2
2,2,3,4
3,4,5,6
4,6,7,8
5,8,9,10
6,10,11,0
*MATERIAL,NAME=WATER
*DENSITY
1000.
*FLUID CONSTANTS
4217.,1750.E-6,273.
*ELSET,ELSET=E1
1,6
*ELSET,ELSET=E2
2
*ELSET,ELSET=E3
3
*ELSET,ELSET=E4
4
*ELSET,ELSET=E5
5
*FLUID SECTION,ELSET=E1,TYPE=CHANNEL INOUT,MATERIAL=WATER
*FLUID SECTION,ELSET=E2,TYPE=CHANNEL SLUICE GATE,MANNING,MATERIAL=WATER
10.,0.005,0.8,,3
*FLUID SECTION,ELSET=E3,TYPE=CHANNEL SLUICE OPENING,MANNING,MATERIAL=WATER
10.,0.005,0.1,0.,0.01,2
*FLUID SECTION,ELSET=E4,TYPE=CHANNEL STRAIGHT,MANNING,MATERIAL=WATER
10.,0.005,49.8,0.,0.01,2
*FLUID SECTION,ELSET=E5,TYPE=CHANNEL RESERVOIR,MANNING,MATERIAL=WATER
10.,0.005,0.1,0.,0.01,2
*BOUNDARY
10,2,2,2.7
*BOUNDARY,MASS FLOW
1,1,1,60000.
```

```
*STEP
*HEAT TRANSFER,STEADY STATE
*DLOAD
EALL,GRAV,9.81,0.,0.,-1.
*NODE PRINT,NSET=NALL
U
*END STEP
```

It is one of the examples in the CalculiX test suite. The channel is made up of six 3-node network elements (type D) in one long line. The nodes have fictitious coordinates. They do not enter the calculations, however, they will be listed in the .frd file. For a proper visualization with CalculiX GraphiX it may be advantageous to use the correct coordinates. As usual in networks, the final node of the entry and exit element have the label zero. The material is water and is characterized by its density, heat capacity and dynamic viscosity. Next, the elements are stored in appropriate sets (by using *ELSET) for the sake of referencing in the *FLUID SECTION card.

The structure of the channel becomes apparent when analyzing the *FLUID SECTION cards: upstream there is a sluice gate, downstream there is a large reservoir and both are connected by a straight channel. Like most upstream elements the sluice gate actually consists of two elements: the actual sluice gate element and a sluice opening element. This is because, although the gate fixes the water depth at its lower end, this water depth may be overrun by a backwater curve controlled by the downstream water level. The sluice gate is described by its width (10 m, which is constant along the channel), a slope of 0.005 (also constant along the channel) and a gate height of 0.8 m. Furthermore, the label of the downstream gate opening element has to be provided as well (3). The sluice opening element has the same width and slope, its length is 0.1 m. If a nonpositive length is provided, the true length is calculated from the nodal coordinates. The angle θ is zero, which means that the cross section is rectangular and not trapezoidal. Since the parameter MANNING has been used on the *FLUID SECTION card, the next parameter (0.01 $m^{-1/3}s$) is the Manning coefficient. Finally, the label of the upstream sluice gate element is given (2). The constants for the straight channel element can be checked in Section 6.6. Important here is the length of 49.8 m. The last element, the reservoir, is again a very short element (length 0.1 m). The length of elements such as the sluice opening or reservoir element, which do not really have a physical length, should be kept small.

Next, the boundary conditions are defined: the reservoir fluid depth is 2.7 m, whereas the mass flow is 60000 kg/s. Network calculations in CalculiX are a special case of steady state heat transfer calculations, therefore the *HEAT TRANSFER, STEADY STATE card is used. The prevailing force is gravity.

When running CalculiX a message appears that there is a hydraulic jump at relative location 0.67 in element 4 (the straight channel element). This is also clear in Figure 40, where the channel has been drawn to scale. The sluice gate is located at x=5 m, the reservoir starts at x=55 m. The bottom of the

channel is shaded black. The water level behind the gate was not prescribed and is one of the results of the calculation: 3.667 m. The water level at the gate is controlled by its height of 0.8 m. A frontwater curve (i.e. a curve controlled by the upstream conditions - the gate) develops downstream and connects to a backwater curve (i.e. a curve controlled by the downstream conditions - the reservoir) by a hydraulic jump at a x-value of 38.5 m. In other words, the jump connects the upstream supercritical flow to the downstream subcritical flow. The critical depth is illustrated in the figure by a dashed line. It is the depth for which the Froude number is 1: critical flow.

In channel flow, the degrees of freedom for the mechanical displacements are reserved for the mass flow, the water depth and the critical depth, respectively. Therefore, the option U underneath the *NODE PRINT card will lead to exactly this information in the .dat file. The same information can be stored in the .frd file by selecting MF, DEPT and HCRI underneath the *NODE FILE card.

5.14 Cantilever beam using beam elements

Previously, a thick cantilever beam was modeled with volume elements. In the present section quadratic beam elements are used for a similar exercise (Section 6.2.27). Beam elements are easy to define: they consist of three nodes on a line. Internally, they are expanded into volumetric elements. There are two types of beam elements: B32 elements, which are expanded into C3D20 elements, and B32R (reduced integration) elements, which are expanded into C3D20R elements. Based on the results in the present section, the B32R element is highly recommended. The B32 element, on the other hand, should be avoided especially if section forces are needed.

The first cantilever beam which is looked at is 100 mm long and has a square cross section of 2 x 2 mm^2. The axis of the beam is along the global z-direction. This beam is modeled with just one element and loaded at its end by a unit force in x-direction, Figure 41. We are interested in the stresses at integration point a and at node b, the section forces at the beam's fixed end, and the displacement in x at the free end. The location of the integration point a is at $x = -1/\sqrt{3}$, $y = 1/\sqrt{3}$ and $z = 50(1 + 1/\sqrt{3})$, the nodal coordinates of b are $x = -1$, $y = 1$ and $z = 100$ [18]. The material is isotropic linear elastic with a Young's modulus of 100,000 MPa and a Poisson's ratio of 0.3.

The input deck for this example is very similar to the simplebeam.inp example in the test suite (Figure 42).

The stresses at the integration points are obtained by a *EL PRINT card, the stresses at the nodes by the OUTPUT=3D option (default) on the *EL FILE card, whereas for the section forces the SECTION FORCES option on the same card is used (this option is mutually exclusive with the OUTPUT=3D option). The displacements are best obtained in the non-expanded view, i.e. using the OUTPUT=2D option. This means that for the present results the example had to be run twice: once with the OUTPUT=3D option and once with the SECTION FORCES option.

The results are summarized in Table 3. The $\{\mathrm{mm}, \mathrm{N}, \mathrm{s}, \mathrm{K}\}$ system is used.

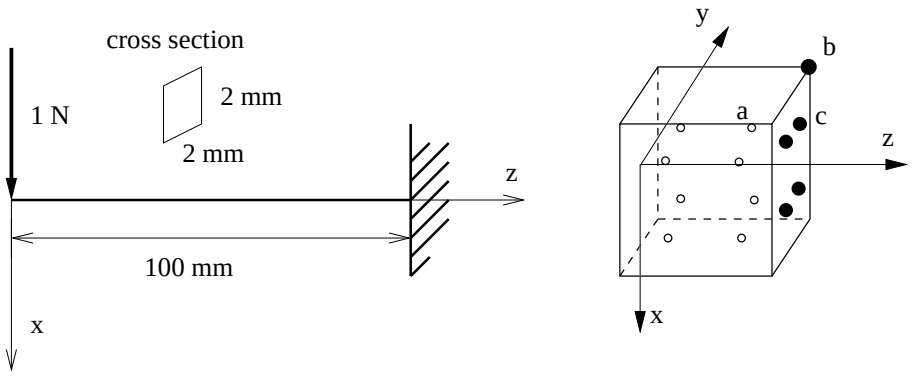


Figure 41: Geometry of the beam

```
**
**   Structure: cantilever beam, one element
**   Test objective: B32R elements.
**
*NODE,NSET=Nall
1,  0,  0,  0
2,  0,  0,  50
3,  0,  0,  100
*ELEMENT,TYPE=B32R,ELSET=EAll
1,1,2,3
*BOUNDARY
3,1,6
*MATERIAL,NAME=ALUM
*ELASTIC
1E5,.3
*BEAM SECTION,ELSET=EAll,MATERIAL=ALUM,SECTION=RECT
2.,2.
1.d0,0.d0,0.d0
*STEP
*STATIC
*CLOAD
1,1,1.
*EL PRINT,ELSET=Eall
S
*NODE FILE
U
*EL FILE,SECTION FORCES
***EL FILE,OUTPUT=3D
S
*END STEP
```

Figure 42: Input deck for the beam

The reference results are analytical results using simple beam theory [58]. The agreement is overwhelming. The stresses at the integration points match exactly, so do the extrapolated normal stresses to the nodes. The shear stresses need special attention. For a beam the shear stress varies parabolically across the section. A quadratic volumetric element can simulate only a linear stress variation across the section. Therefore, the parabolic variation is approximated by a constant shear stress across the section. Since the reduced integration points (at $\pm 1/\sqrt{3}$) happen to be points at which the parabolic stress variation attains its mean value the values at the integration points are exact! The extrapolated values to the nodes take the same constant value and are naturally wrong since the exact value at the corners is zero.

The section forces are obtained by

1. calculating the stresses at the integration points (inside the element, such as integration point a)
2. extrapolating those stresses to the corner nodes (such as node b)
3. calculating the stresses at the middle nodes by interpolation between the adjacent corner nodes
4. interpolating the stresses at all nodes within a section face onto the reduced integration points within the face (such as integration point c, using the shape functions of the face)
5. integrating these stresses numerically.

As shown by Table 3 this procedure yields the correct section forces for the square beam.

The displacements at the beam tip are off by 10 %. The deformation of a beam subject to a shear force at its end is third order, however, the C3D20R element can only simulate a quadratic behavior. The deviation is reduced to 2.4 % by using 5 elements (Table 4). Notice that integration point a is now closer to the fixation (same position is before but in the element adjacent to the fixation).

The same beam was now subjected to a torque of 1 Nmm at its free end. The results are summarized in Table 5.

The torque is matched perfectly, the torsion at the end of the beam (u_y is the displacement in y-direction at the corresponding node of node b) is off by 15 % [58]. The shear stresses at node b are definitely not correct (there is no shear stress at a corner node), however, the integration of the values interpolated from the nodes at the facial integration points yields the exact torque! Using more elements does not change the values in Table 5.

The same exercise is now repeated for a circular cross section (radius = 1 mm, same length, boundary conditions and material data as for the rectangular cross section). For such a cross section the vertex nodes of the element lie at $x, y = \pm 0.7071, \pm 0.7071$, whereas the middle nodes lie at $x, y = 0, \pm 1$ and $x, y = \pm 1, 0$. The integration points are located at $x, y = \pm 0.5210$. The results

Table 3: Results for the square section beam subject to bending (1 element).

result	value	reference
$\sigma_{zz}(a)$	34.151	34.151
$\sigma_{xz}(a)$	-0.25	-0.25
F_{xx}	-1.	-1.
M_{yy}	100.	100.
$\sigma_{zz}(b)$	75.	75.
$\sigma_{xz}(b)$	-0.25	0.
u_x	2.25	2.50

Table 4: Results for the square section beam subject to bending (5 elements).

result	value	reference
$\sigma_{zz}(a)$	41.471	41.471
$\sigma_{xz}(a)$	-0.25	-0.25
F_{xx}	-1.	-1.
M_{yy}	100.	100.
$\sigma_{zz}(b)$	75.	75.
$\sigma_{xz}(b)$	-0.25	0.
u_x	2.44	2.50

Table 5: Results for the square section beam subject to torsion (1 element).

result	value	reference
$\sigma_{xz}(a)$	-0.21651	-
$\sigma_{yz}(a)$	-0.21651	-
M_{zz}	1.	1.
$\sigma_{xz}(b)$	-0.375	0
$\sigma_{yz}(b)$	-0.375	0
u_y	$9.75 \cdot 10^{-4}$	$1.1525 \cdot 10^{-3}$

Table 6: Results for the circular section beam subject to bending (1 element).

result	value	reference
$\sigma_{zz}(a)$	34.00	52.26
$\sigma_{xz}(a)$	-0.322	-0.318
F_{xx}	-0.99996	-1.
M_{yy}	58.7	100.
$\sigma_{zz}(b)$	62.8	90.03
$\sigma_{xz}(b)$	-0.322	-0.318
u_x	2.91	4.24

Table 7: Results for the circular section beam subject to bending (5 elements).

result	value	reference
$\sigma_{zz}(a)$	59.77	63.41
$\sigma_{xz}(a)$	-0.322	-0.318
F_{xx}	-0.99996	-1.
M_{yy}	102.	100.
$\sigma_{zz}(b)$	109.	90.03
$\sigma_{xz}(b)$	-0.322	-0.318
u_x	3.86	4.24

for bending with just one element are shown in Table 6 and with 5 elements in Table 7.

For just one element the shear stress is quite close to the analytical value, leading to a even better match of the shear force. This is remarkable an can only be explained by the fact that the cross area of the piecewise quadratic approximation of the circular circumference is smaller and exactly compensates the slightly higher shear stress. A similar effect will be noticed for the torque. The normal stress, however, is far off at the integration points as well as at the nodes leading to a bending moment which is way too small. The same applies to the deformation in x-direction. Using five elements leads to a significant improvement: the bending moment is only 2 % off, the deformation at the free end 9 %. Here again one can argue that the deformation is of cubic order, whereas a quadratic element can only simulate a quadratic change. Using more elements consequently improves the results.

The results for a torque applied to a circular cross section beam is shown in Table 8 (1 element; the results for 5 elements are identical).

Again, it is remarkable that the torque is perfectly matched, although the shear stress at the integration points is 6 % off. This leads to shear values at the vertex nodes which are 19 % off. Interpolation to the facial integration points yields shear stresses of -0.305 MPa. Integration of these stresses finally leads to

Table 8: Results for the circular section beam subject to torsion (1 element).

result	value	reference
$\sigma_{xz}(a)$	-0.309	-0.331
$\sigma_{yz}(a)$	-0.309	-0.331
M_{zz}	0.999994	1.
$\sigma_{xz}(b)$	-0.535	-0.450
$\sigma_{yz}(b)$	-0.535	-0.450
u_y	$1.54 \cdot 10^{-3}$	$1.66 \cdot 10^{-3}$

the perfect torque values. The torsion angle at the end of the beam is 7 %off.

Summarizing, one can state that the use of C3D20R elements leads to quite remarkable results:

- For a rectangular cross section:
  - the section forces are correct
  - the stresses at the integration points are correct
  - the displacements for bending are correct, provided enough elements are used
  - the torsion angle is somewhat off (15 %).
- For a circular cross section:
  - the shear force and torque section forces are correct
  - the bending moment is correct if enough elements are used
  - the displacements for bending are correct, provided enough elements are used
  - the torsion angle is somewhat off (7 %).

It is generally recommended to calculate the stresses from the section forces. The only drawback is the C3D20R element may lead to hourglassing, leading to weird displacements. However, the mean of the displacements across the cross section is usually fine. An additional problem which can arise is that nonlinear geometric calculations may not converge due to this hourglassing. This is remedied in CalculiX by slightly perturbing the coordinates of the expanded nodes (by about 0.1 %).

A similar exercise was performed for the B32 element, however, the results were quite discouraging. The section forces were, especially for bending, way off.

5.15 Reinforced concrete cantilever beam

Purpose of this exercise is to calculate the stresses in a reinforced concrete cantilever beam due to its own weight. Special issues in this type of problem are the treatment of the structure as a composite and the presence of a compression-only material (the concrete).

The input deck runs like:

```
*NODE, NSET=Nall
       1,1.000000000000e+01,0.000000000000e+00,0.000000000000e+00
...
*ELEMENT, TYPE=S8R, ELSET=Eall
     1,      1,      2,      3,      4,      5,      6,      7,      8
     2,      2,      9,     10,      3,     11,     12,     13,      6
...
** Names based on left
*NSET,NSET=Nleft
49,
50,
52,
** Names based on right
*NSET,NSET=Nright
1,
4,
8,
*MATERIAL,NAME=COMPRESSION_ONLY
*USER MATERIAL,CONSTANTS=2
  1.4e10,        1.e5
*DENSITY
2350.
*MATERIAL,NAME=STEEL
*ELASTIC
210000.e6,.3
*DENSITY
7800.
*SHELL SECTION,ELSET=Eall,COMPOSITE
.09,,COMPRESSION_ONLY
.01,,STEEL
.1,,COMPRESSION_ONLY
.1,,COMPRESSION_ONLY
.1,,COMPRESSION_ONLY
.1,,COMPRESSION_ONLY
.1,,COMPRESSION_ONLY
.1,,COMPRESSION_ONLY
.1,,COMPRESSION_ONLY
.1,,COMPRESSION_ONLY
.1,,COMPRESSION_ONLY
```

```
*BOUNDARY
Nleft,1,6
*STEP,NLGEOM
*STATIC
1.,1.
*DLOAD
Eall,GRAV,9.81,0.,0.,-1.
*NODE FILE
U
*EL FILE
S
*END STEP
```

The beam has a cross section of 1 x 1 m^2 and a length of 10 m. The density of concrete is 2350 kg/m^3, whereas the density of steel is 7800 kg/m^3. The Young's moduli are 14000 MPa and 210000 MPa, respectively. Steel is provided only on the top of the beam (tension side of the beam) at a distance of 9.5 cm from the upper surface. Its layer thickness is 1 cm (in reality the steel is placed within the concrete in the form of bars. The modeling as a thin layer is an approximation. One has to make sure that the complete section of the bars equals the section of the layer). Using the composite feature available for shell structures significantly simplifies the input. Notice that this feature is not (yet) available for beam elements. Consequently the beam was modeled as a plate with a width of 1 m and a length of 10 m. Underneath the *SHELL SECTION card the thickness of the layers and their material is listed, starting at the top of the beam. The direction (from top to bottom) is controlled by the direction of the normal on the shell elements (which is controlled by the order in which the elements' nodes are listed underneath the *ELEMENT card). In a composite shell there are two integration points across each layer. Use of the S8R element is mandatory. In order to capture the location of the neutral axis several layers were used to model the concrete part of the section (in total 10 layers for the concrete and 1 for the steel).

Concrete cannot sustain tension whereas it is largely linear elastic under pressure. This can be modeled with the COMPRESSION_ONLY material model. In CalculiX this is an example of a user material. The name of user materials has to start with a fixed character set, in this case "COMPRESSION_ONLY". The remaining 64 characters (a material name can be at most 80 characters long) can be freely chosen. In the present input deck no extra characters were selected. Choosing extra characters is needed if more than 1 compression-only material is present (in order to distinguish them). The "COMPRESSION_ONLY" material is characterized by 2 constants, the first is Young's modulus, the second is the maximum tensile stress the user is willing to allow, in our case 0.1 MPa (SI-units are used).

Using simple beam theory ([56]) leads to a tensile stress of 152.3 MPa in the steel and a maximum compressive stress of 7.77 MPa at the lower edge of the concrete. The finite element calculation (Figure 43) predicts 152 MPa and

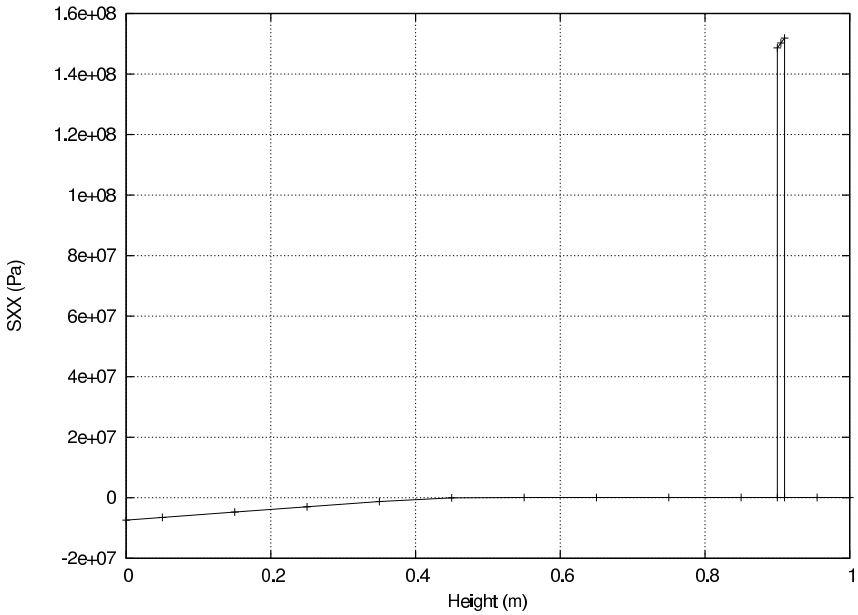


Figure 43: Axial stress across the height of the beam at the fixed end

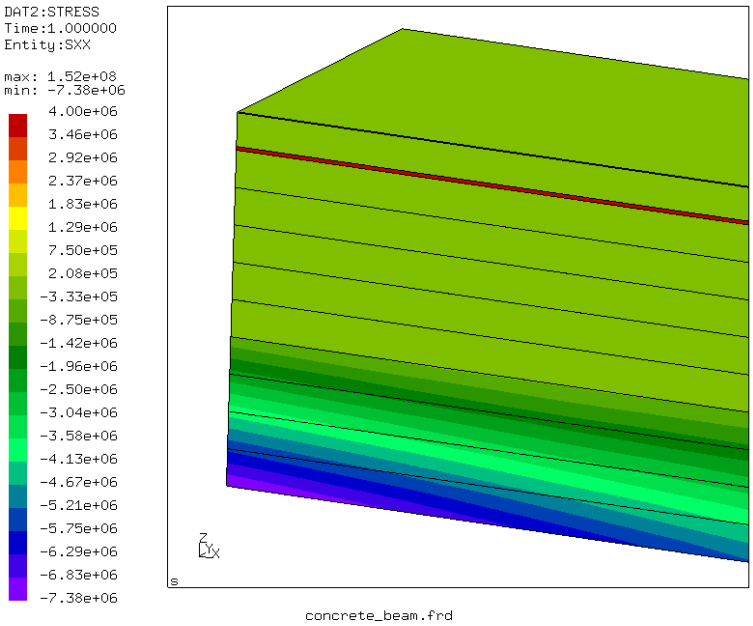


Figure 44: Axial stress across the height of the beam at the fixed end

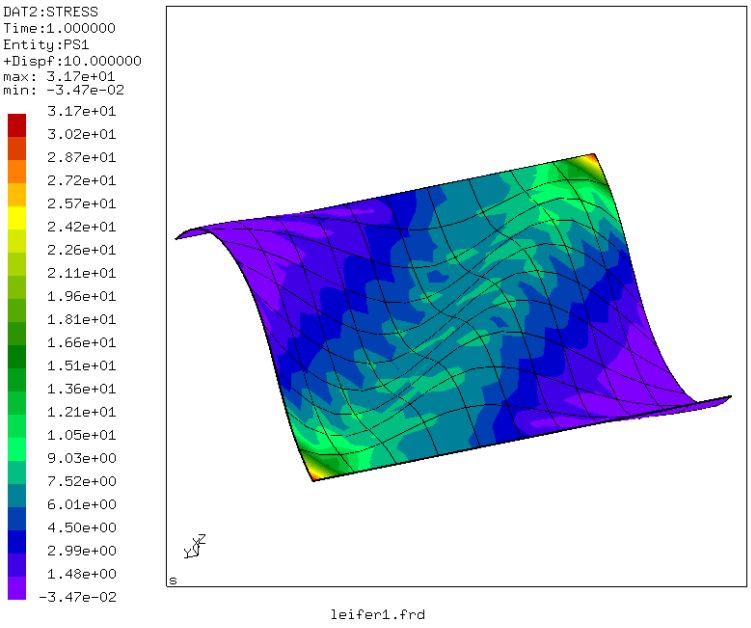


Figure 45: Maximum principal stress in the deformed sheet

7.38 MPa, respectively, which is quite close. In CalculiX, the graphical output of composite structures is always expanded into three dimensions. In Figure 44 one notices the correct dimension of the composite and the high tensile stresses in the thin steel layer.

5.16 Wrinkling of a thin sheet

The input decks for this problem can be found in the test suite as leifer1.inp and leifer2.inp. It was first devised by J. Leifer in 2003. The structure is a thin square sheet with an edge length of 229 mm and a thickness of 0.0762 mm. It is fixed on one side and moved parallel to this side on the opposite side by 1 mm. Young's modulus and Poisson's coefficient are 3790 MPa and 0.38, respectively. Experimental evidence points to the creation of wrinkles due to this shear deformation.

Here, two approaches are described to simulate this experiment. In both cases the sheet is simulated using quadratic shell elements. In the first simulation (leifer1) the material is considered as a linear elastic isotropic material, and wrinkling occurs due to natural buckling processes in the sheet. To enhance this buckling, the coordinates in the direction perpendicular to the sheet (this is the z-direction in our simulation) are slightly perturbed in a aleatoric way (look at the coordinates in the input deck to verify this). Furthermore, the simulation is performed in a dynamic procedure starting with very small time

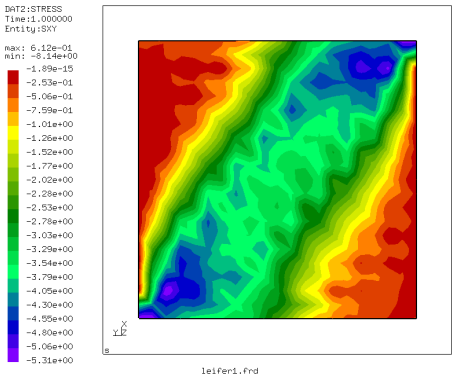


Figure 46: Shear stress in the isotropic simulation

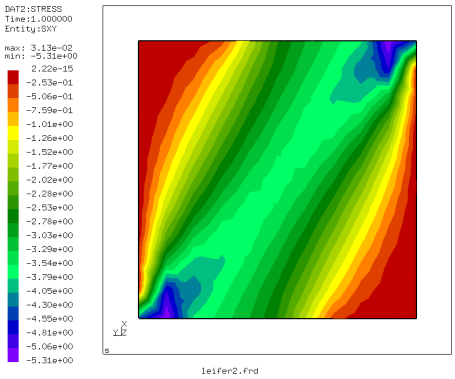


Figure 47: Shear stress in the tension-only simulation

steps. Figure 45 shows the maximum principal stress in the deformed sheet (the edge at x=0 was fixed, the edge at x=229 was moved 1 mm in negative y-direction). One nicely notices the wrinkles. A look at the smallest principal stress shows that there are virtually no pressure stresses in the sheet: they were removed by buckling. A disadvantage of this kind of simulation is the very long computational time (336 increments for a step time of 1!).

The absence of pressure stress points to a second way of obtaining the correct stress distribution: instead of simulating the material as isotropic, one can use a tension-only material model (leifer2). This has the advantage that convergence is much faster (small computational times). Figures 46 and 47 compare the shear stress of both simulations: they match quite nicely (the shear stress distribution in an isotropic simulation without wrinkling is totally different). The same applies to the other stress components. The use of a tension-only material, however, does not lead to out-of-plane deformations. Here, wrinkling can only

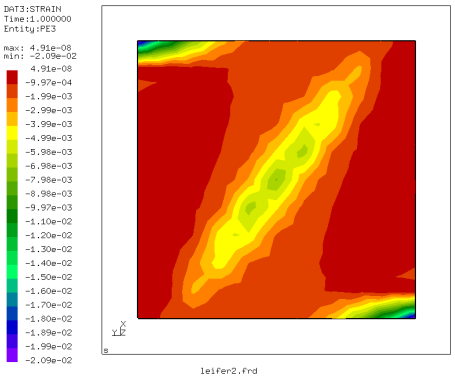


Figure 48: Minimum principal strain in the tension-only simulation

be derived indirectly by looking at the smallest principal strain (Figure 48). The large negative values point to the existence of wrinkles.

6 Theory

The finite element method is basically concerned with the determination of field variables. The most important ones are the stress and strain fields. As basic measure of strain in CalculiX the Lagrangian strain tensor E is used for elastic media, the Eulerian strain tensor e is used for deformation plasticity and the deviatoric elastic left Cauchy-Green tensor is used for incremental plasticity. The Lagrangian strain satisfies ([20]):

$$E_{KL} = (U_{K,L} + U_{L,K} + U_{M,K}U_{M,L})/2, \quad K, L, M = 1, 2, 3 \tag{1}$$

where U_K are the displacement components in the material frame of reference and repeated indices imply summation over the appropriate range. In a linear analysis, this reduces to the familiar form:

$$E_{KL} = (U_{K,L} + U_{L,K})/2, \quad K, L = 1, 2, 3. \tag{2}$$

The Eulerian strain satisfies ([20]):

$$e_{kl} = (u_{k,l} + u_{l,k} - u_{m,k}u_{m,l})/2, \quad k, l, m = 1, 2, 3 \tag{3}$$

where u_k are the displacements components in the spatial frame of reference.

Finally, the deviatoric elastic left Cauchy-Green tensor is defined by ([66]):

$$\bar{b}^e_{kl} = J^{e-2/3} x^e_{k,K} x^e_{l,K} \tag{4}$$

where J^e is the elastic Jacobian and $x^e_{k,K}$ is the elastic deformation gradient. The above formulas apply for Cartesian coordinate systems.

The stress measure consistent with the Lagrangian strain is the second Piola-Kirchhoff stress S. This stress, which is internally used in CalculiX for all applications (the so-called total Lagrangian approach, see [9]), can be transformed into the first Piola-Kirchhoff stress P (the so-called engineering stress, a non-symmetric tensor) and into the Cauchy stress t (true stress). All CalculiX input (e.g. distributed loading) and output is in terms of true stress. In a tensile test on a specimen with length L the three stress measures are related by:

$$t = P/(1-\epsilon) = S/(1-\epsilon)^2 \tag{5}$$

where ϵ is the engineering strain defined by

$$\epsilon = dL/L. \tag{6}$$

6.1 Node Types

There are three node types:

- 1D fluid nodes. These are nodes satisfying at least one of the following conditions:
  - nodes belonging to 1D network elements (element labels starting with D)
  - reference nodes in *FILM cards of type forced convection (label: F*FC).
  - reference nodes in *DLOAD cards of type nodal pressure (label: P*NP).
- 3D fluid nodes. These are nodes belonging to 3D fluid elements (element labels starting with F)
- structural nodes. Any nodes not being 1D fluid nodes nor 3D fluid nodes.

It is not allowed to create equations between nodes of different types.

6.2 Element Types

6.2.1 Eight-node brick element (C3D8 and F3D8)

The C3D8 element is a general purpose linear brick element, fully integrated (2x2x2 integration points). The shape functions can be found in [39]. The node numbering follows the convention of Figure 49 and the integration points are numbered according to Figure 50. This latter information is important since element variables printed with the *EL PRINT keyword are given in the integration points.

Although the structure of the element is straightforward, it should not be used in the following situations:

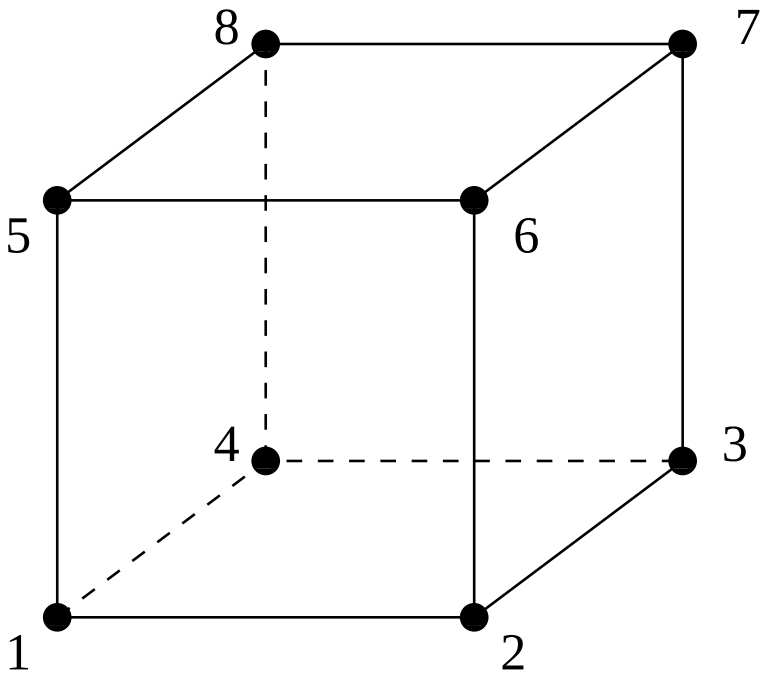


Figure 49: 8-node brick element

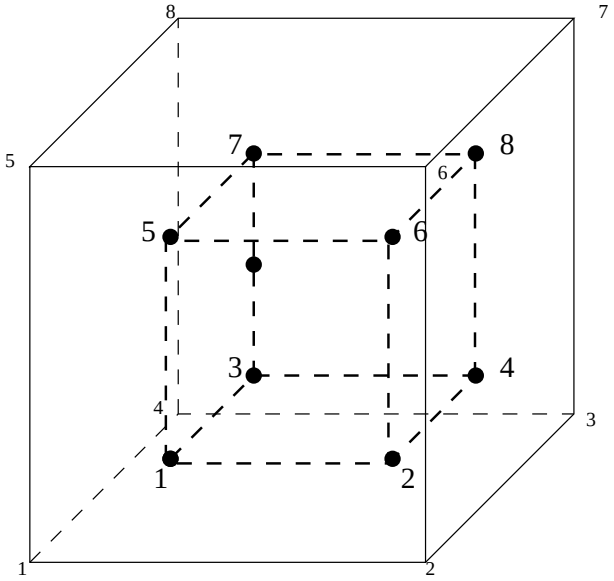


Figure 50: 2x2x2 integration point scheme in hexahedral elements

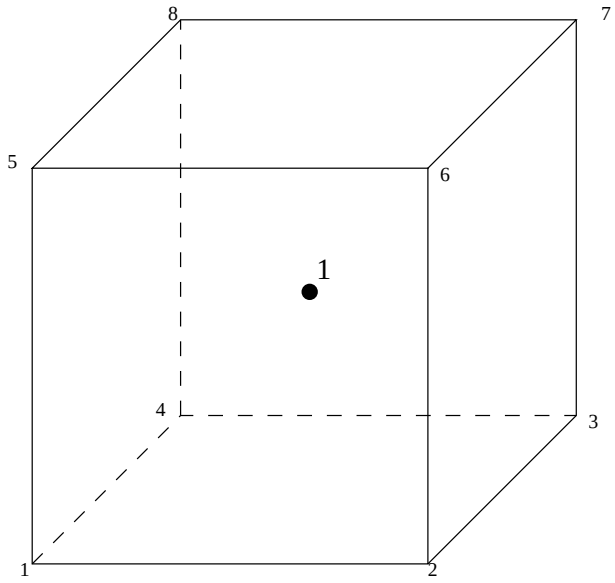


Figure 51: 1x1x1 integration point scheme in hexahedral elements

- due to the full integration, the element will behave badly for isochoric material behavior, i.e. for high values of Poisson's coefficient or plastic behavior.
- the element tends to be too stiff in bending, e.g. for slender beams or thin plates under bending. [78].

The F3D8 element is the corresponding fluid element.

6.2.2 Eight-node brick element with reduced integration (C3D8R)

The C3D8R element is a general purpose linear brick element, with reduced integration (1 integration point). The shape functions are the same as for the C3D8 element and can be found in [39]. The node numbering follows the convention of Figure 49 and the integration point is shown in Fig 51.

Due to the reduced integration, the locking phenomena observed in the C3D8 element do not show. However, the element exhibits other shortcomings:

- The element tends to be not stiff enough in bending.
- Stresses, strains.. are most accurate in the integration points. The integration point of the C3D8R element is located in the middle of the element. Thus, small elements are required to capture a stress concentration at the boundary of a structure.
- There are 12 spurious zero energy modes leading to massive hourglassing: this means that the correct solution is superposed by arbitrarily large

displacements corresponding to the zero energy modes. Thus, the displacements are completely wrong. Since the zero energy modes do no lead to any stresses, the stress field is still correct. In practice, the C3D8R element is not very useful without hourglass control. Starting with version 2.3 hourglass control is automatically activated for this element (using the theory in [23]), thus alleviating this issue.

6.2.3 Incompatible mode eight-node brick element (C3D8I)

The incompatible mode eight-node brick element is an improved version of the C3D8-element. In particular, shear locking is removed and volumetric locking is much reduced. This is obtained by supplementing the standard shape functions with so-called bubble functions, which have a zero value at all nodes and nonzero values in between. In CalculiX, the version detailed in [72] has been implemented. The C3D8I element should be used in all instances, in which linear elements are subject to bending. Although the quality of the C3D8I element is far better than the C3D8 element, the best results are usually obtained with quadratic elements (C3D20 and C3D20R). Notice that the C3D8I element cannot be used in *DYNAMIC calculations (the extra three degrees of freedom of the C3D8I element do not have a mass associated. This leads to a singular mass matrix).

6.2.4 Twenty-node brick element (C3D20)

The C3D20 element is a general purpose quadratic brick element (3x3x3 integration points). The shape functions can be found in [39]. The node numbering follows the convention of Figure 52 and the integration scheme is given in Figure 53.

This is an excellent element for linear elastic calculations. Due to the location of the integration points, stress concentrations at the surface of a structure are well captured. However, for nonlinear calculations the elements exhibits the same disadvantages as the C3D8 element, albeit to a much lesser extent:

- due to the full integration, the element will behave badly for isochoric material behavior, i.e. for high values of Poisson's coefficient or plastic behavior.
- the element tends to be too stiff in bending, e.g. for slender beams or thin plates under bending. [78].

6.2.5 Twenty-node brick element with reduced integration (C3D20R)

The C3D20R element is a general purpose quadratic brick element, with reduced integration (2x2x2 integration points). The shape functions can be found in [39]. The node numbering follows the convention of Figure 52 and the integration scheme is shown in Figure 50.

The element behaves very well and is an excellent general purpose element (if you are setting off for a long journey and you are allowed to take only one

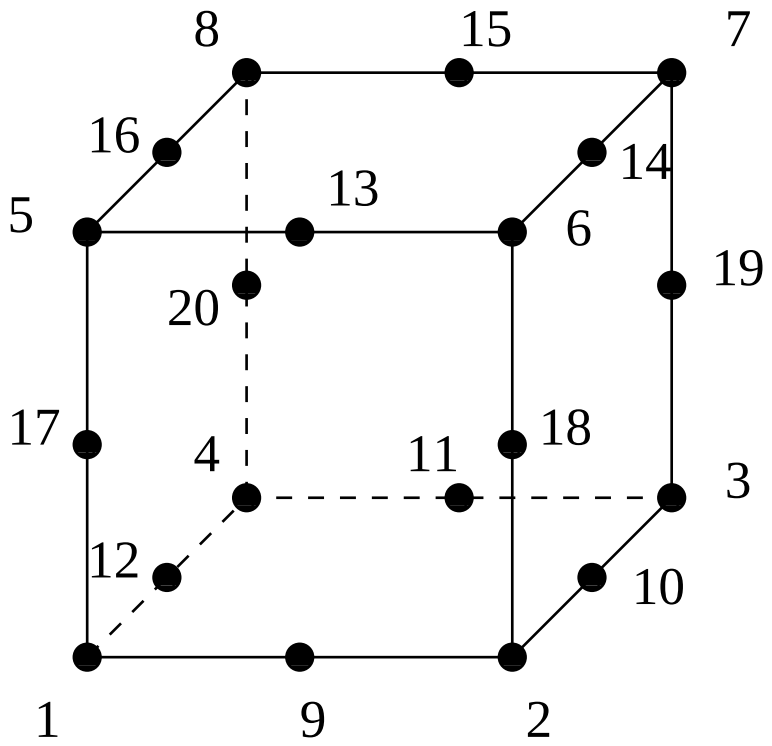


Figure 52: 20-node brick element

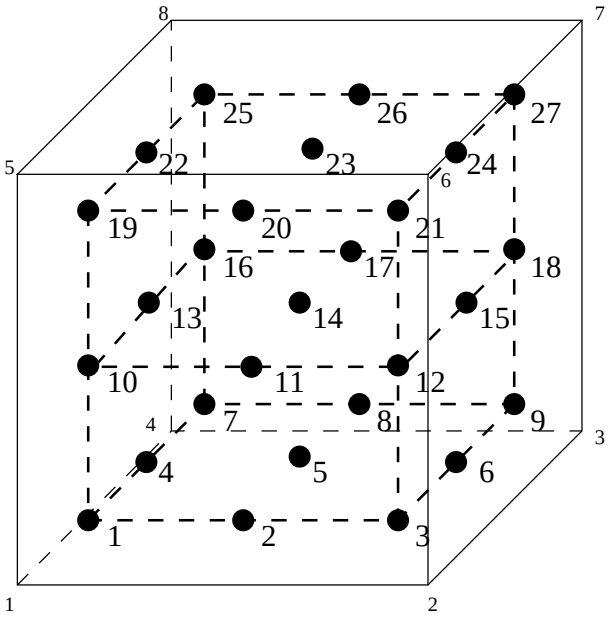


Figure 53: 3x3x3 integration point scheme in hexahedral elements

element type with you, that's the one to take). It also performs well for isochoric material behavior and in bending and rarely exhibits hourglassing despite the reduced integration (hourglassing generally occurs when not enough integration points are used for numerical integration and spurious modes pop up resulting in crazy displacement fields but correct stress fields). The reduced integration points are so-called superconvergent points of the element [7]. Just two caveats:

- the integration points are about one quarter of the typical element size away from the boundary of the element, and the extrapolation of integration point values to the nodes is trilinear. Thus, high stress concentrations at the surface of a structure might not be captured if the mesh is too coarse.

- all quadratic elements cause problems in node-to-face contact calculations, because the nodal forces in the vertex nodes equivalent to constant pressure on an element side (section 6.11.2) are zero or have the opposite sign of those in the midside nodes. This problem seems to be solved if face-to-face contact is used.

6.2.6 Four-node tetrahedral element (C3D4 and F3D4)

The C3D4 is a general purpose tetrahedral element (1 integration point). The shape functions can be found in [78]. The node numbering follows the convention of Figure 54.

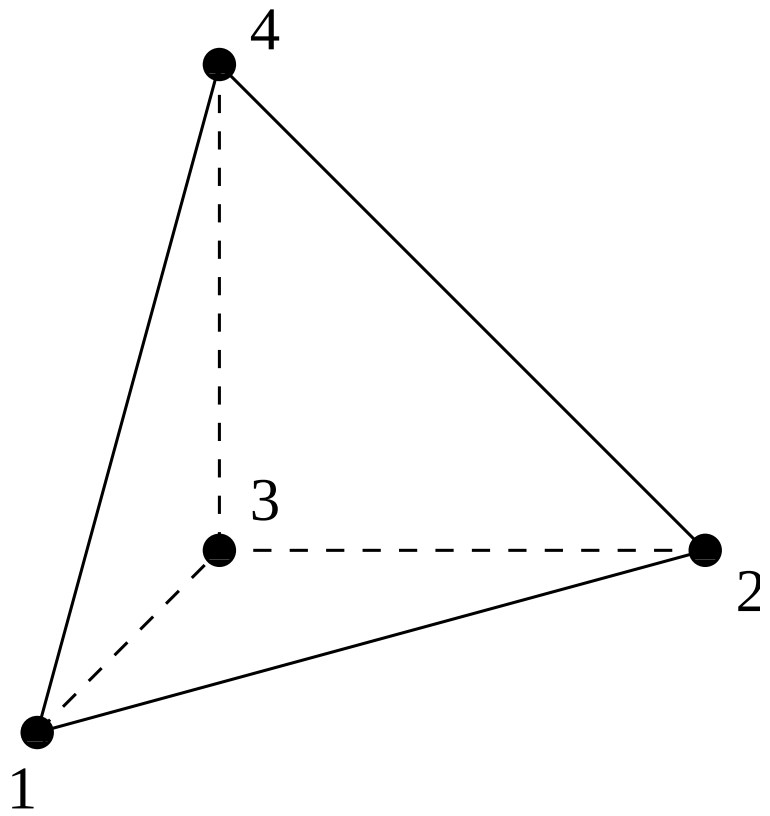


Figure 54: 4-node tetrahedral element

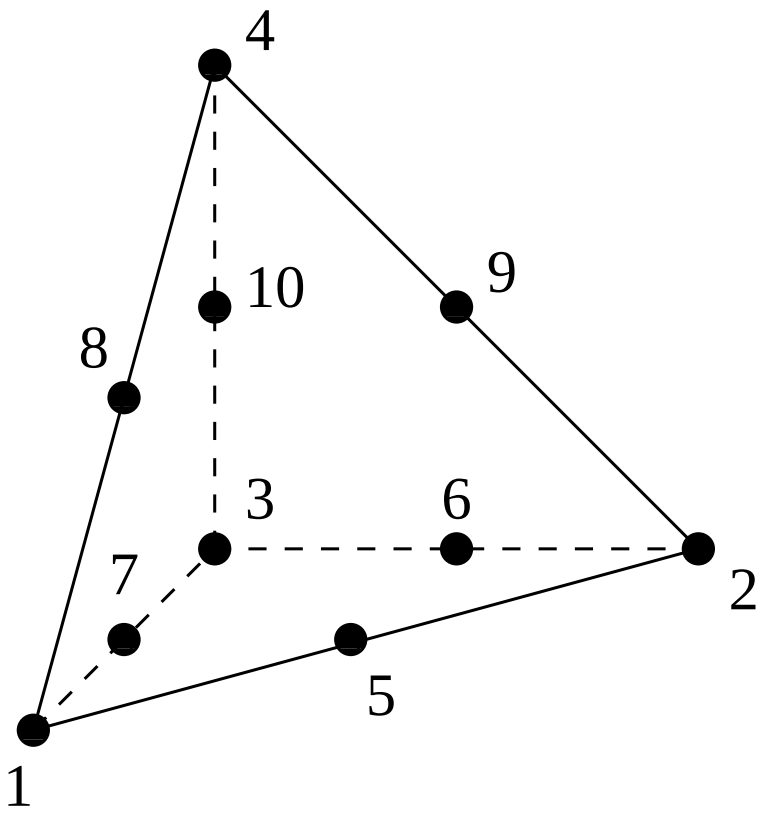


Figure 55: 10-node tetrahedral element

This element is included for completeness, however, it is not suited for structural calculations unless a lot of them are used (the element is too stiff). Please use the 10-node tetrahedral element instead.

The F3D4 element is the corresponding fluid element.

6.2.7 Ten-node tetrahedral element (C3D10)

The C3D10 element is a general purpose tetrahedral element (4 integration points). The shape functions can be found in [78]. The node numbering follows the convention of Figure 55.

The element behaves very well and is a good general purpose element, although the C3D20R element yields still better results for the same number of degrees of freedom. The C3D10 element is especially attractive because of the existence of fully automatic tetrahedral meshers.

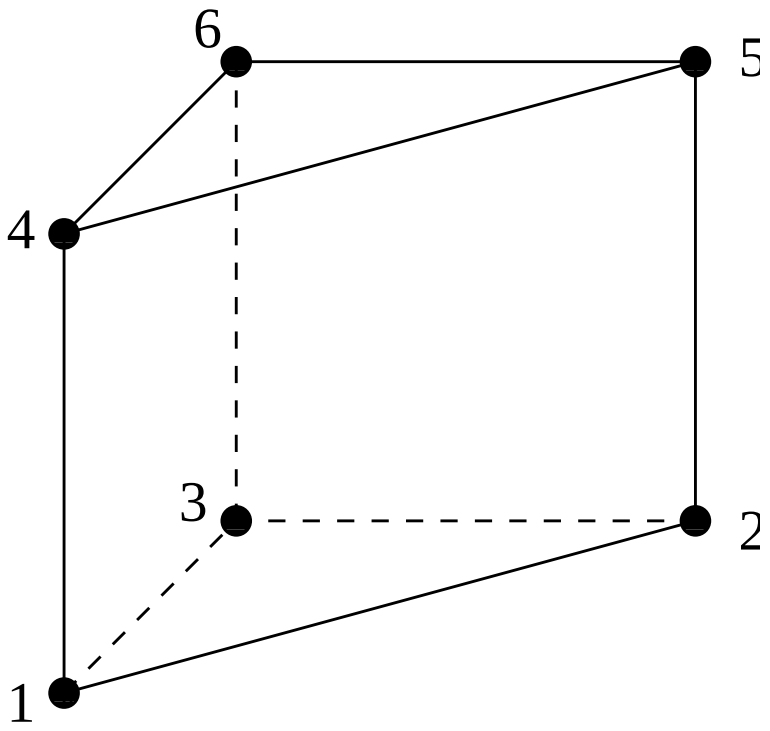


Figure 56: 6-node wedge element

6.2.8 Six-node wedge element (C3D6 and F3D6)

The C3D6 element is a general purpose wedge element (2 integration points). The shape functions can be found in [1]. The node numbering follows the convention of Figure 56.

This element is included for completeness, however, it is probably not very well suited for structural calculations unless a lot of them are used. Please use the 15-node wedge element instead.

The F3D6 element is the corresponding fluid element.

6.2.9 Fifteen-node wedge element (C3D15)

The C3D15 element is a general purpose wedge element (9 integration points). The shape functions can be found in [1]. The node numbering follows the convention of Figure 57.

The element behaves very well and is a good general purpose element, although the C3D20R element yields still better results for the same number of degrees of freedom. The wedge element is often used as fill element in "automatic" hexahedral meshers.

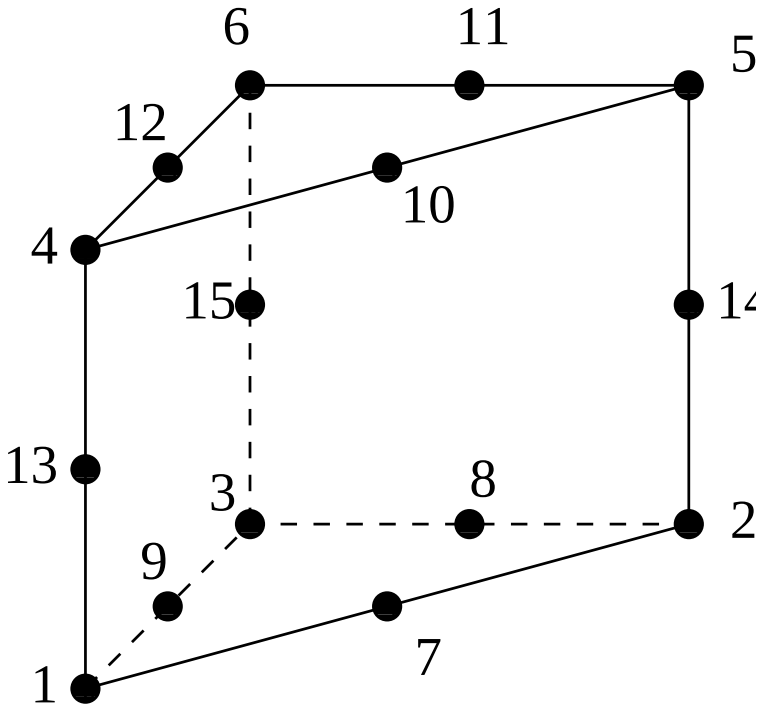


Figure 57: 15-node wedge element

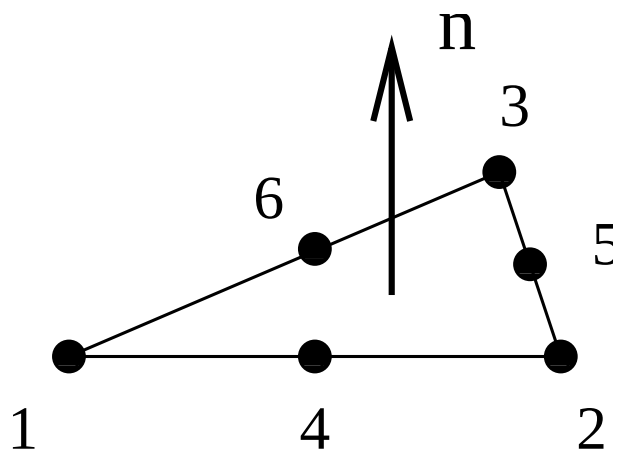


Figure 58: 6-node triangular element

6.2.10 Three-node shell element (S3)

This is a general purpose linear triangular shell element. For the node numbering and the direction of the normal to the surface the reader is referred to the quadratic six-node shell element (S6) in Figure 58 (just drop the middle nodes).

In CalculiX, three-node shell elements are expanded into three-dimensional C3D6 wedge elements. The way this is done can be derived from the analogous treatment of the S6-element in Figure 59 (again, drop the middle nodes). For more information on shell elements the reader is referred to the eight-node shell element S8.

6.2.11 Four-node shell element (S4 and S4R)

This is a general purpose linear 4-sided shell element. For the node numbering and the direction of the normal to the surface the reader is referred to the quadratic eight-node shell element (S8) in Figure 60 (just drop the middle nodes).

In CalculiX, S4 and S4R four-node shell elements are expanded into three-dimensional C3D8I and C3D8R elements, respectively. The way this is done can be derived from the analogous treatment of the S8-element in Figure 61 (again, drop the middle nodes). For more information on shell elements the reader is referred to the eight-node shell element S8.

6.2.12 Six-node shell element (S6)

This is a general purpose triangular shell element. The node numbering and the direction of the normal to the surface is shown in Figure 58.

In CalculiX, six-node shell elements are expanded into three-dimensional wedge elements. The way in which this is done is illustrated in Figure 59. For

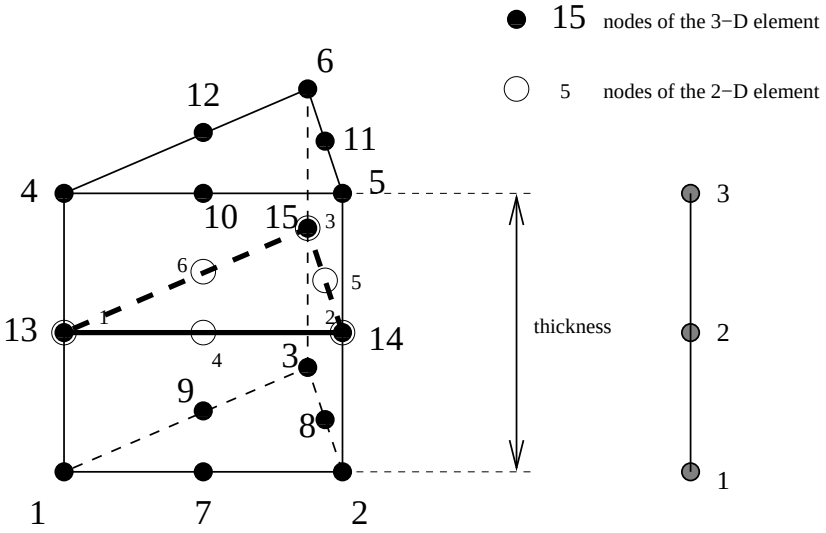


Figure 59: Expansion of a 2D 6-node element into a 3D wedge element

more information on shell elements the reader is referred to the eight-node shell element in the next section.

6.2.13 Eight-node shell element (S8 and S8R)

This element is a general purpose 4-sided shell element. The node numbering and the direction of the normal to the surface is shown in Figure 60.

In CalculiX, quadratic shell elements are automatically expanded into 20-node brick elements. The way this is done is illustrated in Figure 61. For each shell node three new nodes are generated according to the scheme on the right of Figure 61. With these nodes a new 20-node brick element is generated: for a S8 element a C3D20 element, for a S8R element a C3D20R element.

Since a shell element can be curved, the normal to the shell surface is defined in each node separately. For this purpose the *NORMAL keyword card can be used. If no normal is defined by the user, it will be calculated automatically by CalculiX based on the local geometry.

If a node belongs to more than one shell element, all, some or none of the normals on these elements in the node at stake might have been defined by the user (by means of *NORMAL). The failing normals are determined based on the local geometry (notice, however, that for significantly distorted elements it may not be possible to determine the normal; this particularly applies to elements in which the middle nodes are way off the middle position). The number of normals is subsequently reduced using the following procedure. First, the element with the lowest element number with an explicitly defined normal in this set, if any, is taken and used as reference. Its normal is defined as reference normal and the element is stored in a new subset. All other elements of the same type in

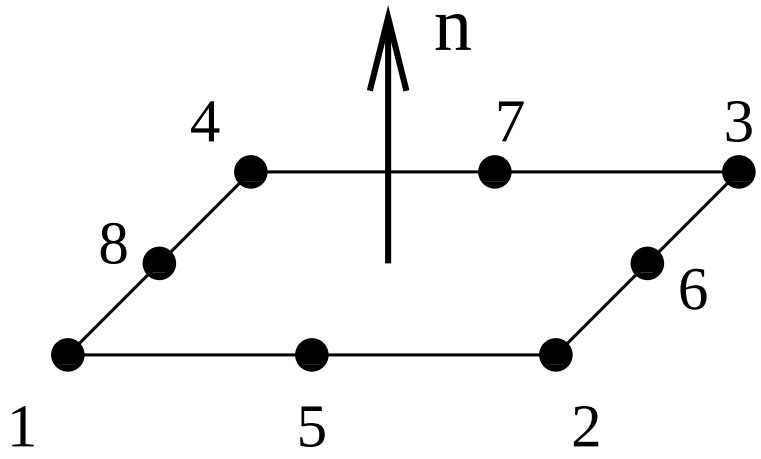


Figure 60: 8-node quadratic element

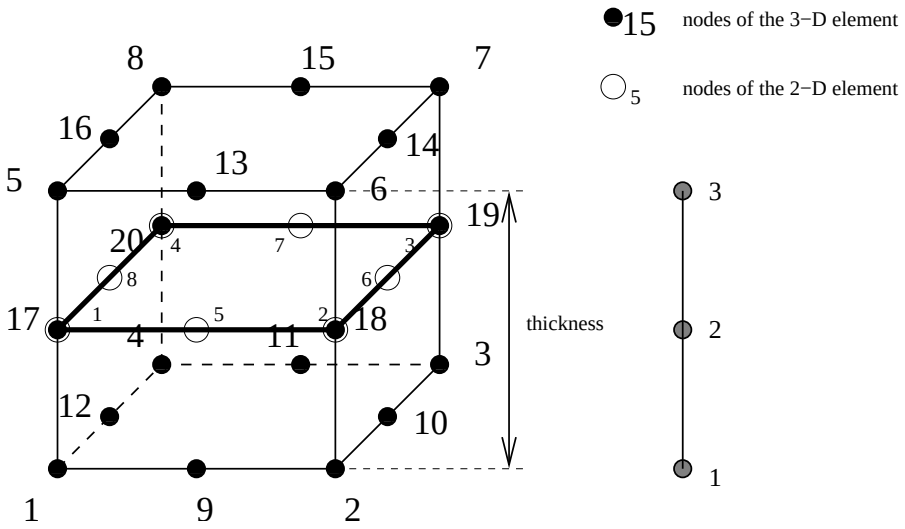


Figure 61: Expansion of a 2D 8-node element into a 3D brick element

the set for which the normal has an angle smaller than 0.5° with the reference normal and which have the same local thickness and offset are also included in this subset. The elements in the subset are considered to have the same normal, which is defined as the normed mean of all normals in the subset. This procedure is repeated for the elements in the set minus the subset until no elements are left with an explicitly defined normal. Now, the element with the lowest element number of all elements left in the set is used as reference. Its normal is defined as reference normal and the element is stored in a new subset. All other elements left in the set for which the normal has an angle smaller than 20° with the reference normal and which have the same local thickness and offset are also included in this subset. The normed mean of all normals in the subset is assigned as new normal to all elements in the subset. This procedure is repeated for the elements left until a normal has been defined in each element.

This procedure leads to one or more normals in one and the same node. If only one normal is defined, this node is expanded once into a set of three new nodes and the resulting three-dimensional expansion is continuous in the node. If more than one normal is defined, the node is expanded as many times as there are normals in the node. To assure that the resulting 3D elements are connected, the newly generated nodes are considered as a knot. A knot is a rigid body which is allowed to expand uniformly. This implies that a knot is characterized by seven degrees of freedom: three translations, three rotations and a uniform expansion. Graphically, the shell elements partially overlap (Figure 62).

Consequently, a node leads to a knot if

- the direction of the local normals in the elements participating in the node differ beyond a given amount. Notice that this also applies to neighboring elements having the inverse normal. Care should be taken that the elements in plates and similar structures are oriented in a consistent way to avoid the generation of knots and the induced nonlinearity.
- several types of elements participate (e.g. shells and beams).
- the thickness is not the same in all participating elements.
- the offset is not the same in all participating elements.
- a rotation or a moment is applied in the node (only for dynamic calculations)

In CalculiX versions prior to and including version 2.7 a knot was also introduced as soon as the user applied a rotation or a moment to a node. In static calculations, starting with version 2.8 this type of loading is handled by using mean rotation MPC's (cf. Section 8.7.1). The mean rotation MPC's are generated automatically, so the user does not have to take care of that. It generally leads to slightly better results then by use of knots. However, the use of mean rotation MPC's prohibits the application of drilling moments, i.e. moments about an axis perpendicular to a shell surface. Similarly, no drilling rotation should be prescribed, unless all rotational degrees of freedom are set to

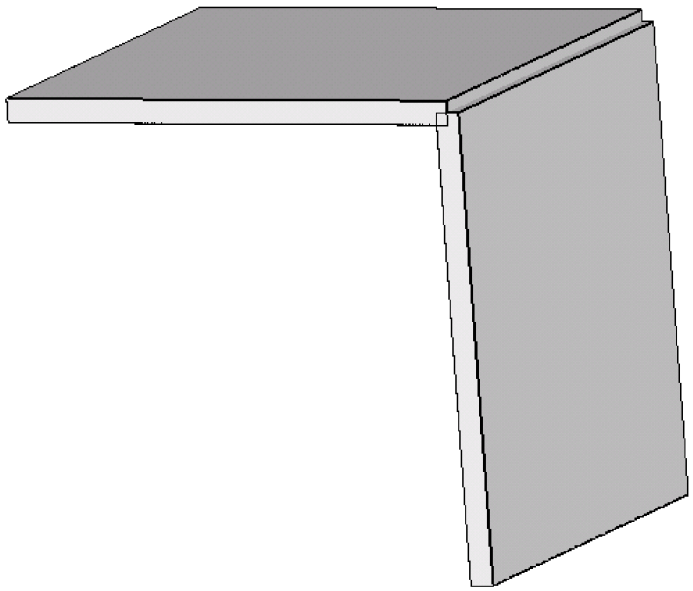


Figure 62: Overlapping shell elements at a knot

zero in the node. If the shell surface is not aligned along the global coordinate directions, prescribing a moment or rotation aboun an axis perpendicular to the drilling direction may require the definition of a local coordinate system. Also note that the rotation in a mean rotation MPC should not exceed 90 degrees.

Beam and shell elements are always connected in a stiff way if they share common nodes. This, however, does not apply to plane stress, plane strain and axisymmetric elements. Although any mixture of 1D and 2D elements generates a knot, the knot is modeled as a hinge for any plane stress, plane strain or axisymmetric elements involved in the knot. This is necessary to account for the special nature of these elements (the displacement normal to the symmetry plane and normal to the radial planes is zero for plane elements and axisymmetric elements, respectively).

The translational node of the knot (cfr REF NODE in the *RIGID BODY keyword card) is the knot generating node, the rotational node is extra generated.

The thickness of the shell element can be defined on the *SHELL SECTION keyword card. It applies to the complete element. Alternatively, a nodal thickness in each node separately can be defined using *NODAL THICKNESS. In that way, a shell with variable thickness can be modeled. Thicknesses defined by a *NODAL THICKNESS card take precedence over thicknesses defined by a *SHELL SECTION card. The thickness always applies in normal direction. The *SHELL SECTION card is also used to assign a material to the shell elements and is therefore indispensable.

The offset of a shell element can be set on the *SHELL SECTION card. Default is zero. The unit of the offset is the local shell thickness. An offset of 0.5 means that the user-defined shell reference surface is in reality the top surface of the expanded element. The offset can take any real value. Consequently, it can be used to define composite materials. Defining three different shell elements using exactly the same nodes but with offsets -1, 0 and 1 (assuming the thickness is the same) leads to a three-layer composite.

However, due to the introduction of a knot in every node of such a composite, the deformation is usually too stiff. Therefore, a different method has been coded to treat composites. Right now, it can only be used for 8-node shells with reduced integration (S8R). Instead of defining as many shells as there are layers the user only defines one shell element, and uses the option COMPOSITE on the *SHELL SECTION card. Underneath the latter card the user can define as many layers as needed. Internally, the shell element is expanded into only one 3-D brick element but the number of integration points across the thickness amounts to twice the number of layers. During the calculation the integration points are assigned the material properties appropriate for the layer they belong to. In the .dat file the user will find the displacements of the global 3-D element and the stresses in all integration points (provided the user has requested the corresponding output using the *NODE PRINT and *EL PRINT card). In the .frd file, however, each layer is expanded independently and the displacements and stresses are interpolated/extrapolated accordingly (no matter whether the parameter OUTPUT=3D was used). The restrictions on this kind of composite

element are right now:

- can only be used for S8R elements
- reaction forces (RF) cannot be requested in the .frd file.
- the use of *NODAL THICKNESS is not allowed

The treatment of the boundary conditions for shell elements is straightforward. The user can independently fix any translational degree of freedom (DOF 1 through 3) or any rotational DOF (DOF 4 through 6). Here, DOF 4 is the rotation about the global or local x-axis, DOF 5 about the global or local y-axis and DOF 6 about the global or local z-axis. Local axes apply if the transformation (*TRANSFORM) has been defined, else the global system applies. A hinge is defined by fixing the translational degrees of freedom only. Recall that it is not allowed to constrain a rotation about the drilling axis on a shell, unless the rotations about all axes in the node are set to zero.

For an internal hinge between 1D or 2D elements the nodes must be doubled and connected with MPC's. The connection between 3D elements and all other elements (1D or 2D) is always hinged.

Point forces defined in a shell node are modified if a knot is generated (the reference node of the rigid body is the shell node). If no knot is generated, the point load is divided among the expanded nodes according to a 1/2-1/2 ratio for a shell mid-node and a 1/6-2/3-1/6 ratio for a shell end-node. Concentrated bending moments or torques are defined as point loads (*CLOAD) acting on degree four to six in the node. Their use generates a knot in the node.

Distributed loading can be defined by the label P in the *DLOAD card. A positive value corresponds to a pressure load in normal direction.

In addition to a temperature for the reference surface of the shell, a temperature gradient in normal direction can be specified on the *TEMPERATURE card. Default is zero.

Concerning the output, nodal quantities requested by the keyword *NODE PRINT are stored in the shell nodes. They are obtained by averaging the nodal values of the expanded element. For instance, the value in local shell node 1 are obtained by averaging the nodal value of expanded nodes 1 and 5. Similar relationships apply to the other nodes, in 6-node shells:

- shell node 1 = average of expanded nodes 1 and 4
- shell node 2 = average of expanded nodes 2 and 5
- shell node 3 = average of expanded nodes 3 and 6
- shell node 4 = average of expanded nodes 7 and 10
- shell node 5 = average of expanded nodes 8 and 11
- shell node 6 = average of expanded nodes 9 and 12

In 8-node shells:

- shell node 1 = average of expanded nodes 1 and 5
- shell node 2 = average of expanded nodes 2 and 6
- shell node 3 = average of expanded nodes 3 and 7
- shell node 4 = average of expanded nodes 4 and 8
- shell node 5 = average of expanded nodes 9 and 13
- shell node 6 = average of expanded nodes 10 and 14
- shell node 7 = average of expanded nodes 11 and 15
- shell node 8 = average of expanded nodes 12 and 16

Element quantities, requested by *EL PRINT are stored in the integration points of the expanded elements.

Default storage for quantities requested by the *NODE FILE and *EL FILE is in the expanded nodes. This has the advantage that the true three-dimensional results can be viewed in the expanded structure, however, the nodal numbering is different from the shell nodes. By selecting OUTPUT=2D the results are stored in the original shell nodes. The same averaging procedure applies as for the *NODE PRINT command.

In thin structures two words of caution are due: the first is with respect to reduced integration. If the aspect ratio of the beams is very large (slender beams, aspect ratio of 40 or more) reduced integration will give you far better results than full integration. However, due to the small thickness hourglassing can readily occur, especially if point loads are applied. This results in displacements which are widely wrong, however, the stresses and section forces are correct. Usually also the mean displacements across the section are fine. If not, full integration combined with smaller elements might be necessary. Secondly, thin structures can easily exhibit large strains and/or rotations. Therefore, most calculations require the use of the NLGEOM parameter on the *STEP card.

6.2.14 Three-node plane stress element (CPS3)

This element is very similar to the three-node shell element. Figures 58 and 59 apply (just drop the middle nodes). For more information on plane stress elements the reader is referred to the section on CPS8 elements.

6.2.15 Four-node plane stress element (CPS4 and CPS4R)

This element is very similar to the eight-node shell element. Figures 60 and 61 apply (just drop the middle nodes). The CPS4 and CPS4R elements are expanded into C3D8 and C3D8R elements, respectively. For more information on plane stress elements the reader is referred to the section on CPS8 elements.

6.2.16 Six-node plane stress element (CPS6)

This element is very similar to the six-node shell element. Figures 58 and 59 apply. For more information on plane stress elements the reader is referred to the next section.

6.2.17 Eight-node plane stress element (CPS8 and CPS8R)

The eight node plane stress element is a general purpose plane stress element. It is actually a special case of shell element: the structure is assumed to have a symmetry plane parallel to the x-y plane and the loading only acts in-plane. In general, the z-coordinates are zero. Just like in the case of the shell element, the plane stress element is expanded into a C3D20 or C3D20R element. Figures 60 and 61 apply. From the above premises the following conclusions can be drawn:

- The displacement in z-direction of the midplane is zero. This condition is introduced in the form of SPC's. MPC's must not be defined in z-direction!
- The displacements perpendicular to the z-direction of nodes not in the midplane is identical to the displacements of the corresponding nodes in the midplane.
- The normal is by default (0,0,1)
- The thickness can vary. It can be defined in the same way as for the shell element, except that the *SOLID SECTION card is used instead of the *SHELL SECTION card.
- Different offsets do not make sense.
- Point loads are treated in a similar way as for shells.

The use of plane stress elements can also lead to knots, namely, if the thickness varies in a discontinuous way, or if plane stress elements are combined with other 1D or 2D elements such as axisymmetric elements. The connection with the plane stress elements, however, is modeled as a hinge.

Distributed loading in plane stress elements is different from shell distributed loading: for the plane stress element it is in-plane, for the shell element it is out-of-plane. Distributed loading in plane stress elements is defined on the *DLOAD card with the labels P1 up to P4. The number indicates the face as defined in Figure 63.

If a plane stress element is connected to a structure consisting of 3D elements the motion of this structure in the out-of-plane direction (z-direction) is not restricted by its connection to the 2D elements. The user has to take care that any rigid body motion of the structure involving the z-direction is taken care of, if appropriate. This particularly applies to any springs connected to plane stress elements, look at test example spring4 for an illustration.

Notice that structures containing plane stress elements should be defined in the global x-y plane, i.e. z=0 for all nodes.

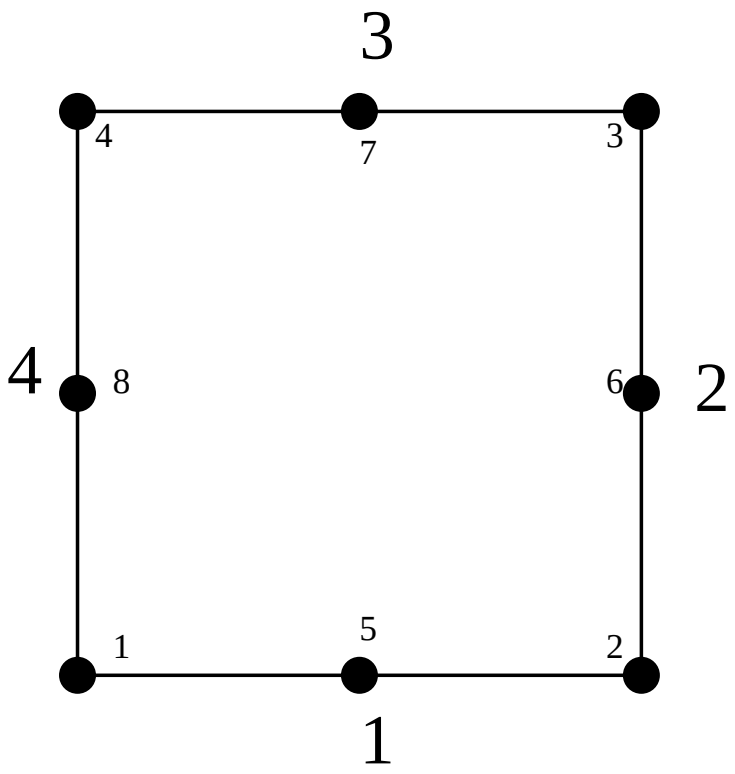


Figure 63: Face numbering for quadrilateral elements

6.2.18 Three-node plane strain element (CPE3)

This element is very similar to the three-node shell element. Figures 58 and 59 apply (just drop the middle nodes). For more information on plane strain elements the reader is referred to the section on CPE8 elements.

6.2.19 Four-node plane strain element (CPE4 and CPE4R)

This element is very similar to the eight-node shell element. Figures 60 and 61 apply (just drop the middle nodes). The CPE4 and CPE4R elements are expanded into C3D8 and C3D8R elements, respectively. For more information on plane strain elements the reader is referred to the section on CPE8 elements.

6.2.20 Six-node plane strain element (CPE6)

This element is very similar to the six-node shell element. Figures 58 and 59 apply. For more information on plane strain elements the reader is referred to the next section.

6.2.21 Eight-node plane strain element (CPE8 and CPE8R)

The eight node plane strain element is a general purpose plane strain element. It is actually a special case of plane stress element: the treatise of Section 6.2.17 also applies here. In addition we have:

- The displacement in z-direction of all nodes (not only the mid-nodes) is zero. This condition is introduced in the form of MPC's, expressing that the displacement in z-direction of nodes not in the midplane is identical to the displacement of the corresponding nodes in the midplane.
- Different thicknesses do not make sense: one thickness applicable to all plane strain elements suffices.

Plane strain elements are used to model a slice of a very long structure, e.g. of a dam.

If a plane strain element is connected to a structure consisting of 3D elements the motion of this structure in the out-of-plane direction (z-direction) is not restricted by its connection to the 2D elements. The user has to take care that any rigid body motion of the structure involving the z-direction is taken care of, if appropriate. This particularly applies to any springs connected to plane strain elements.

Notice that structures containing plane strain elements should be defined in the global x-y plane, i.e. z=0 for all nodes.

6.2.22 Three-node axisymmetric element (CAX3)

This element is very similar to the three-node shell element. Figures 58 and 59 apply (just drop the middle nodes). For more information on axisymmetric elements the reader is referred to the section on CAX8 elements.

6.2.23 Four-node axisymmetric element (CAX4 and CAX4R)

This element is very similar to the eight-node shell element. Figures 60 and 61 apply (just drop the middle nodes). The CAX4 and CAX4R elements are expanded into C3D8 and C3D8R elements, respectively. For more information on axisymmetric elements the reader is referred to the section on CAX8 elements.

6.2.24 Six-node axisymmetric element (CAX6)

This element is very similar to the six-node shell element. Figures 58 and 59 apply. For more information on axisymmetric elements the reader is referred to the next section.

6.2.25 Eight-node axisymmetric element (CAX8 and CAX8R)

This is a general purpose quadratic axisymmetric element. Just as the shell, plane stress and plane strain element it is internally expanded into a C3D20 or C3D20R element according to Figure 61 and the node numbering of Figure 60 applies.

For axisymmetric elements the coordinates of the nodes correspond to the radial direction (first coordinate) and the axial direction (second or y-coordinate). The axisymmetric structure is expanded by rotation about the second coordinate axis, half clockwise and half counterclockwise. The radial direction corresponds to the x-axis in the 3D expansion, the axial direction with the y-axis. The x-y plane cuts the expanded structure in half. The z-axis is perpendicular to the x-y plane such that a right-hand-side axis system is obtained.

The same rules apply as for the plane strain elements, except that in-plane conditions in a plane strain construction now correspond to radial plane conditions in the axisymmetric structure. Expressed in another way, the z-direction in plane strain now corresponds to the circumferential direction in a cylindrical coordinate system with the y-axis as defining axis.

Compared to plane strain elements, the following conditions apply:

- The expansion angle is fixed, its size is 2°. The value on the line beneath the *SOLID SECTION keyword, if any, has no effect.
- The displacements in cylindrical coordinates of all nodes not in the defining plane are identical to the displacements of the corresponding nodes in the defining plane. This is formulated using MPC's.
- Forces act in radial planes. They have to be defined for the complete circumference, i.e. if you apply a force in a node, you first have to sum all forces at that location along the circumference and then apply this sum to the node.
- Concentrated heat fluxes act in radial planes. They have to be defined for the complete circumference.

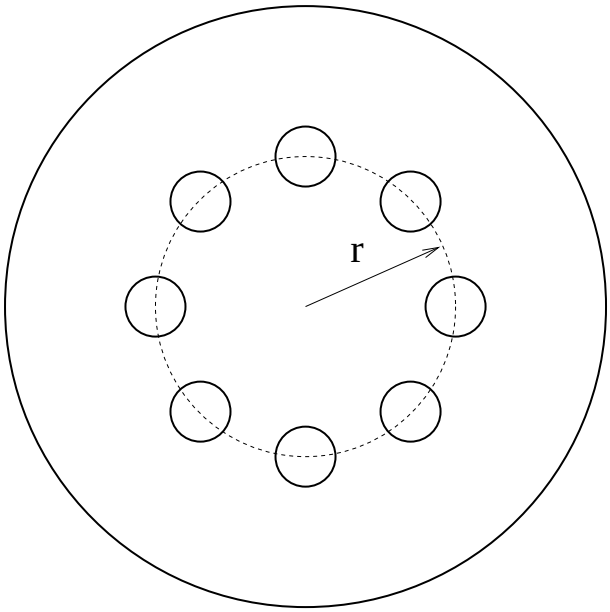


Figure 64: Disk with holes

- Mass flow rates act in radial planes. They have to be defined for the complete circumference.
- For distributed loading Figure 63 applies.

A special application is the combination of axisymmetric elements with plane stress elements to model quasi-axisymmetric structures. Consider a circular disk with holes along the circumference, Figure 64. Assume that the holes take up $k\%$ of the circumferential width, i.e. if the center of the holes is located at a radius r, the holes occupy $2\pi rk/100$. Then, the structure is reduced to a two-dimensional model by simulating the holes by plane stress elements with width $2\pi r(100-k)/100$ and everything else by axisymmetric elements. More sophisticated models can be devised (e.g. taking the volume of the holes into account instead of the width at their center, or adjusting the material properties as well [35]). The point here is that due to the expansion into three-dimensional elements a couple of extra guidelines have to be followed:

- expanded plane stress and axisymmetric elements must have a small thickness to yield good results: in the case of plane stress elements this is because a large thickness does not agree with the plane stress assumption, in the case of axisymmetric elements because large angles yield bad results since the expansion creates only one layer of elements. CalculiX uses an expansion angle of 2°, which amounts to $\pi/90$ radians. Consequently, only $100/180\%$ of the disk is modeled and the thickness of the plane stress

elements is $(100-k)\pi r/9000$. This is done automatically within CalculiX. On the *SOLID SECTION card the user must specify the thickness of the plane stress elements for 360°, i.e. $2\pi r(100-k)/100$.

- the point forces on the axisymmetric elements are to be given for the complete circumference, as usual for axisymmetric elements.
- the point forces on the plane stress elements act on the complete circumference.
- distributed loads are not affected, since they act on areas and/or volumes.

If an axisymmetric element is connected to a structure consisting of 3D elements the motion of this structure in the circumferential direction is not restricted by its connection to the 2D elements. The user has to take care that any rigid body motion of the structure involving the circumferential direction is taken care of, if appropriate. This particularly applies to any springs connected to axisymmetric elements.

Notice that structures containing axisymmetric elements should be defined in the global x-y plane, i.e. z=0 for all nodes.

6.2.26 Two-node beam element (B31 and B31R)

This element is very similar to the three-node beam element. Figures 65 and 66 apply (just drop the middle nodes). The B31 and B31R elements are expanded into C3D8I and C3D8R elements, respectively. Since the C3D8R element has only one integration point in the middle of the element, bending effect cannot be taken into account. Therefore,the B31R element should not be used for bending. For more information on beam elements the reader is referred to the next section.

6.2.27 Three-node beam element (B32 and B32R)

In CalculiX this is the general purpose beam element. The node numbering is shown in Figure 65.

In each node a local Cartesian system $\mathbf{t}-\mathbf{n_1}-\mathbf{n_2}$ is defined. $\mathbf{t}$ is the normalized local tangential vector, $\mathbf{n_1}$ is a normalized vector in the local 1-direction and $\mathbf{n_2}$ is a normalized vector in the local 2-direction, also called the normal. The local directions 1 and 2 are used to expand the beam element into a C3D20 or C3D20R element according to Figure 66.

For each node of the beam element 8 new nodes are generated according to the scheme on the right of Figure 66. These new nodes are used in the definition of the brick element, and their position is defined by the local directions together with the thickness and offset in these directions.

The tangential direction follows from the geometry of the beam element. The normal direction (2-direction) can be defined in two ways:

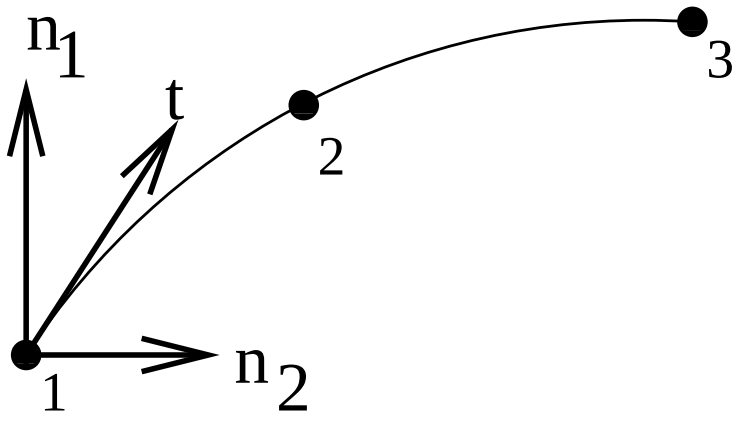


Figure 65: 3-node quadratic beam element/3-node network element

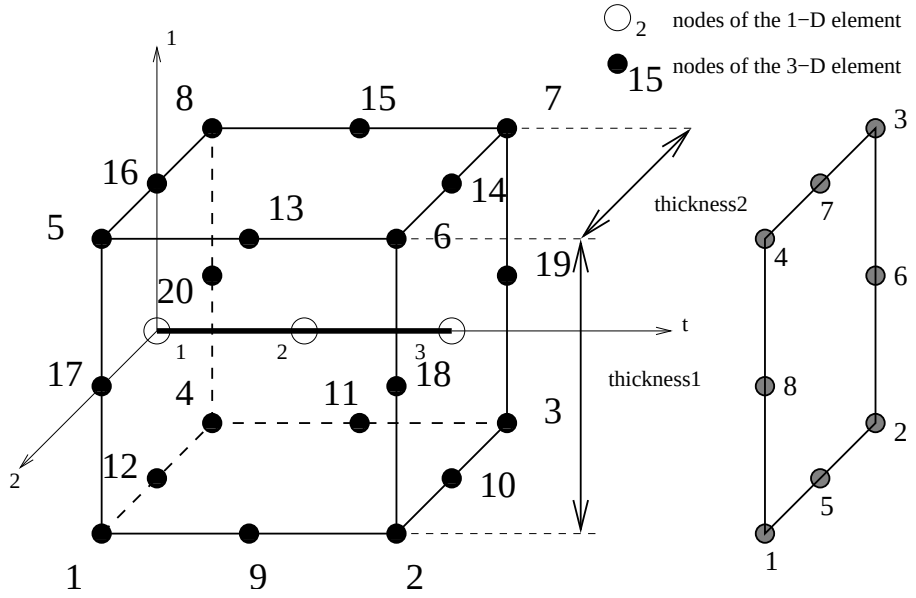


Figure 66: Expansion of a beam element

- either by defining the normal explicitly by using the *NORMAL keyword card.
- if the normal is not defined by the *NORMAL card, it is defined implicitly by $\mathbf{n_2} = \mathbf{t} \times \mathbf{n_1}$

In the latter case, $\mathbf{n_1}$ can be defined either

- explicitly on the *BEAM SECTION card.
- implicitly through the default of (0,0,-1).

If a node belongs to more than one beam element, the tangent and the normal is first calculated for all elements to which the node belongs. Then, the element with the lowest element number in this set for which the normal was defined explicitly using a *NORMAL card is used as reference. Its normal and tangent are defined as reference normal and reference tangent and the element is stored in a new subset. All other elements of the same type in the set for which the normal and tangent have an angle smaller than 0.5° with the reference normal and tangent and which have the same local thicknesses, offsets and sections are also included in this subset. All elements in the subset are considered to have the same normal and tangent. The normal is defined as the normed mean of all normals in the subset, the same applies to the tangent. Finally, the normal is slightly modified within the tangent-normal plane such that it is normal to the tangent. This procedure is repeated until no elements are left with an explicitly defined normal. Then, the element with the lowest element number left in the set is used as reference. Its normal and tangent are defined as reference normal and reference tangent and the element is stored in a new subset. All other elements of the same type in the set for which the normal and tangent have an angle smaller than 20° with the reference normal and tangent and which have the same local thicknesses, offsets and sections are also included in this subset. All elements in the subset are considered to have the same normal and tangent. This normal is defined as the normed mean of all normals in the subset, the same applies to the tangent. Finally, the normal is slightly modified within the tangent-normal plane such that it is normal to the tangent. This procedure is repeated until a normal and tangent have been defined in each element. Finally, the 1-direction is defined by $\mathbf{n_1} = \mathbf{n_2} \times \mathbf{t}$.

If this procedure leads to more than one local coordinate system in one and the same node, all expanded nodes are considered to behave as a knot with the generating node as reference node. Graphically, the beam elements partially overlap (Figure 67).

Consequently, a node leads to a knot if

- the direction of the local normals in the elements participating in the node differ beyond a given amount. Notice that this also applies to neighboring elements having the inverse normal. Care should be taken that the elements in beams are oriented in a consistent way to avoid the generation of knots.

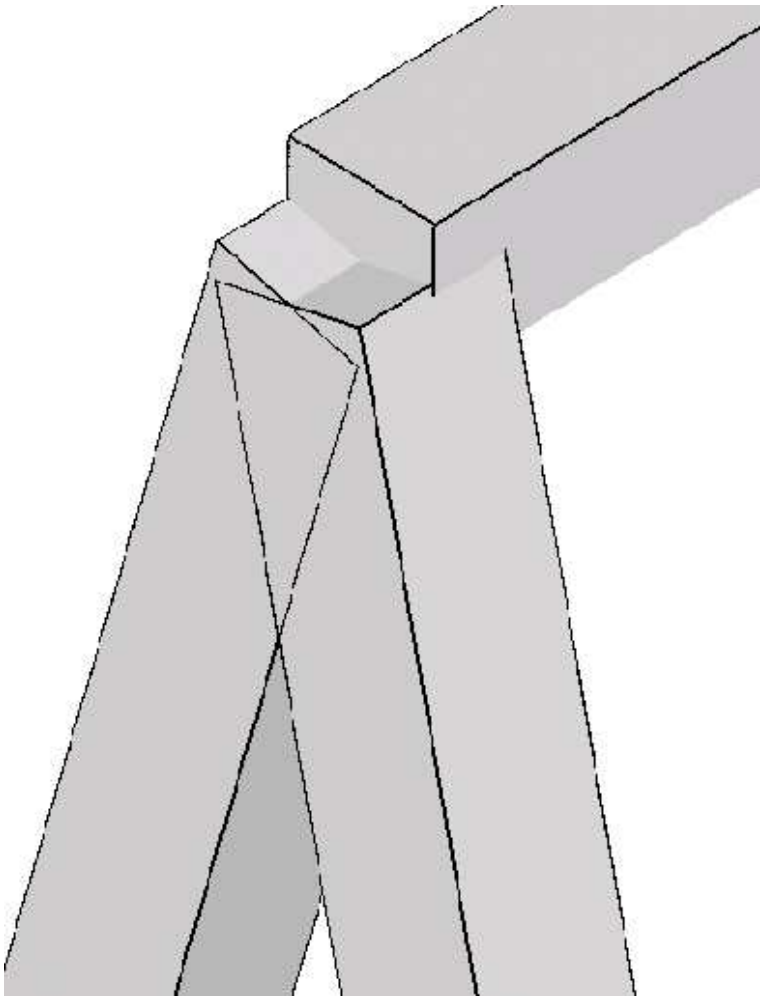


Figure 67: Overlapping beam elements at a knot

- several types of elements participate (e.g. shells and beams).
- the thickness is not the same in all participating elements.
- the offset is not the same in all participating elements.
- the section is not the same in all participating elements.
- a rotation or a moment is applied in the node (only for dynamic calculations)

Similarly to shells applied rotations or moments (bending moments, torques) in static calculations are taken care of by the automatic generation of mean rotation MPC's.

Beam and shell elements are always connected in a stiff way if they share common nodes. This, however, does not apply to plane stress, plane strain and axisymmetric elements. Although any mixture of 1D and 2D elements generates a knot, the knot is modeled as a hinge for any plane stress, plane strain or axisymmetric elements involved in the knot. This is necessary to account for the special nature of these elements (the displacement normal to the symmetry plane and normal to the radial planes is zero for plane elements and axisymmetric elements, respectively).

The section of the beam must be specified on the *BEAM SECTION keyword card. It can be rectangular (SECTION=RECT) or elliptical (SECTION=CIRC). A circular cross section is a special case of elliptical section. For a rectangular cross section the local axes must be defined parallel to the sides of the section, for an elliptical section they are parallel to the minor and major axes of the section. The thickness of a section is the distance between the free surfaces, i.e. for a circular section it is the diameter.

The thicknesses of the beam element (in 1- and 2-direction) can be defined on the *BEAM SECTION keyword card. It applies to the complete element. Alternatively, the nodal thicknesses can be defined in each node separately using *NODAL THICKNESS. That way, a beam with variable thickness can be modeled. Thicknesses defined by a *NODAL THICKNESS card take precedence over thicknesses defined by a *BEAM SECTION card.

The offsets of a beam element (in 1- and 2-direction) can be set on the *BEAM SECTION card. Default is zero. The unit of the offset is the beam thickness in the appropriate direction. An offset of 0.5 means that the user-defined beam reference line lies in reality on the positive surface of the expanded beam (i.e. the surface with an external normal in direction of the local axis). The offset can take any real value. Consequently, it can be used to define composite structures, such as a plate supported by a beam, or a I cross section built up of rectangular cross sections.

The treatment of the boundary conditions for beam elements is straightforward. The user can independently fix any translational degree of freedom (DOF 1 through 3) or any rotational DOF (DOF 4 through 6). Here, DOF 4 is the rotation about the global x-axis, DOF 5 about the global y-axis and DOF 6

about the global z-axis. No local coordinate system should be defined in nodes with constrained rotational degrees of freedom. A hinge is defined by fixing the translational degrees of freedom only.

For an internal hinge between 1D or 2D elements the nodes must be doubled and connected with MPC's. The connection between 3D elements and all other elements (1D or 2D) is always hinged.

Point forces defined in a beam node are not modified if a knot is generated (the reference node is the beam node). If no knot is generated, the point load is divided among the expanded nodes according to a 1/4-1/4-1/4-1/4 ratio for a beam mid-node and a (-1/12)-(1/3)-(-1/12)-(1/3)-(-1/12)-(1/3)-(-1/12)-(1/3) ratio for a beam end-node. Concentrated bending moments or torques are defined as point loads (*CLOAD) acting on degree four to six in the node. Their use generates a knot in the node.

Distributed loading can be defined by the labels P1 and P2 in the *DLOAD card. A positive value corresponds to a pressure load in direction 1 and 2, respectively.

In addition to a temperature for the reference surface of the beam, a temperature gradient in 1-direction and in 2-direction can be specified on the *TEMPERATURE. Default is zero.

Concerning the output, nodal quantities requested by the keyword *NODE PRINT are stored in the beam nodes. They are obtained by averaging the nodal values of the expanded element. For instance, the value in local beam node 1 are obtained by averaging the nodal value of expanded nodes 1, 4, 5 and 8. Similar relationships apply to the other nodes:

- beam node 1 = average of expanded nodes 1,4,5 and 8
- beam node 2 = average of expanded nodes 9,11,13 and 15
- beam node 3 = average of expanded nodes 2,3,6 and 7

Element quantities, requested by *EL PRINT are stored in the integration points of the expanded elements.

Default storage for quantities requested by the *NODE FILE and *EL FILE is in the expanded nodes. This has the advantage that the true three-dimensional results can be viewed in the expanded structure, however, the nodal numbering is different from the beam nodes. By using the OUTPUT=2D parameter in the first step one can trigger the storage in the original beam nodes. The same averaging procedure applies as for the *NODE PRINT command. Section forces can be requested by means of the parameter SECTION FORCES. If selected, the stresses in the beam nodes are replaced by the section forces. They are calculated in a local coordinate system consisting of the 1-direction $\mathbf{n_1}$, the 2-direction $\mathbf{n_2}$ and 3-direction or tangential direction $\mathbf{t}$ (Figure 66). Accordingly, the stress components now have the following meaning:

- xx: Shear force in 1-direction
- yy: Shear force in 2-direction

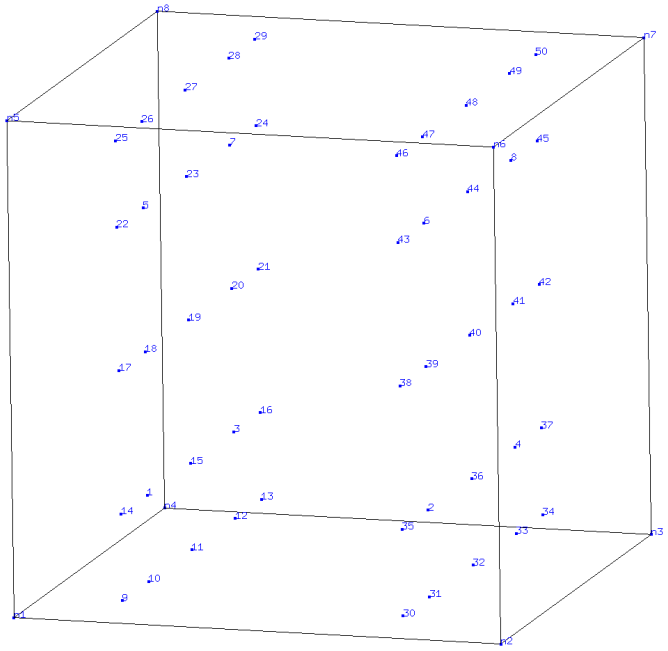


Figure 68: Gauss-Kronrod integration scheme for B32R elements with rectangular cross section

- zz: Normal force
- xy: Torque
- xz: Bending moment about the 2-direction
- yz: Bending moment about the 1-direction

The section forces are calculated by a numerical integration of the stresses over the cross section. To this end the stress tensor is needed at the integration points of the cross section. It is determined from the stress tensors at the nodes belonging to the cross section by use of the shape functions. Therefore, if the section forces look wrong, look at the stresses in the expanded beams (omitting the SECTION FORCES and OUTPUT=2D parameter). The SECTION FORCES parameter automatically triggers the OUTPUT=2D parameter for all results but the stresses.

For all elements except the beam elements the parameter SECTION FORCES has no effect.

In thin structures two words of caution are due: the first is with respect to reduced integration. If the aspect ratio of the shells is very large (slender shells)

reduced integration will give you far better results than full integration. In order to avoid hourglassing a 2x5x5 Gauss-Kronrod integration scheme is used for B32R-elements with a rectangular cross section. This scheme contains the classical Gauss scheme with reduced integration as a subset. The integration point numbering is shown in Figure 68. For circular cross sections the regular reduced Gauss scheme is used. In the rare cases that hourglassing occurs the user might want to use full integration with smaller elements. Secondly, thin structures can easily exhibit large strains and/or rotations. Therefore, most calculations require the use of the NLGEOM parameter on the *STEP card.

6.2.28 Three-node network element (D)

This is a general purpose network element used in forced convection applications. It consists of three nodes: two corner nodes and one midside node. The node numbering is shown in Figure 65. In the corner nodes the only active degrees of freedom are the temperature degree of freedom (degree of freedom 11) and the pressure degree of freedom (degree of freedom 2). These nodes can be used in forced convection *FILM conditions. In the middle node the only active degree of freedom is degree of freedom 1, and stands for the mass flow rate through the element. A positive mass flow rate flows from local node 1 to local node 3, a negative mass flow rate in the reverse direction. It can be defined using a *BOUNDARY card for the first degree of freedom of the midside node of the element. Fluid material properties can be defined using the *MATERIAL, *FLUID CONSTANTS and *SPECIFIC GAS CONSTANT cards and assigned by the *FLUID SECTION card.

network elements form fluid dynamic networks and should not share any node with any other type of element. Basically, analyses involving fluid dynamic networks belong to one of the following two types of calculations:

- Pure thermomechanical calculations. In that case the mass flow in all elements of the network is known and the only unknowns are the temperature (in the network and the structure) and displacements (in the structure). This mode is automatically activated if all mass flows are specified using boundary cards. In that case, pressures in the network are NOT calculated. Furthermore, the type of network element is not relevant and should not be specified.

- Fully coupled calculations involving fluid thermodynamical calculations with structural thermomechanical calculations. This mode is triggered if the mass flow in at least one of the network elements is not known. It requires for each network element the specification of its fluid section type.

The available types of fluid sections are listed in subsection 6.4 and 6.5.

Notice that three-node network elements are one-dimensional and can account for two- or three-dimensional effects in the fluid flow only to a limited degree.

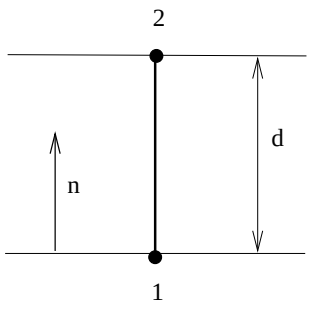


Figure 69: Definition of a GAPUNI element

A special kind of network element is one in which one of the corner nodes is zero (also called a dummy network element). This type is element is used at those locations where mass flow enters or leaves the network. In this case the corner node which is not connected to any other network element gets the label zero. This node has no degrees of freedom. The degree of freedom 1 of the midside node corresponds to the entering or leaving mass flow.

6.2.29 Two-node unidirectional gap element (GAPUNI)

This is a standard gap element defined between two nodes. The clearance d of the gap and its direction $\boldsymbol{n}$ are defined by using the *GAP card. Let the displacement vector of the first node of the GAPUNI element be $\boldsymbol{u_1}$ and the displacement vector of the second node $\boldsymbol{u_2}$. Then, the gap condition is defined by (Figure 69):

$$d + \boldsymbol{n} \cdot (\boldsymbol{u_2} - \boldsymbol{u_1}) \geq 0. \tag{7}$$

6.2.30 Two-node 3-dimensional dashpot (DASHPOTA)

The dashpot element is defined between two nodes (Figure 70). The force in node 2 amounts to:

$$\boldsymbol{F_2} = -c \left[(\boldsymbol{v_2} - \boldsymbol{v_1}) \cdot \frac{(\boldsymbol{x_2} - \boldsymbol{x_1})}{L} \right] \frac{(\boldsymbol{x_2} - \boldsymbol{x_1})}{L} \tag{8}$$

where c is the dashpot coefficient, $\boldsymbol{v}$ is the velocity vector, $\boldsymbol{x}$ is the actual location of the nodes and L is the actual distance between them. Notice that $\boldsymbol{F_1} = -\boldsymbol{F_2}$. Right now, only linear dashpots are allowed, i.e. the dashpot coefficient is constant (i.e. it does not depend on the relative velocity. However, it can depend on the temperature). It is defined using the *DASHPOT keyword card.

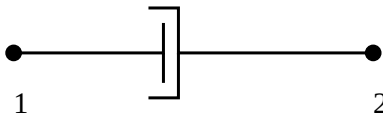


Figure 70: Definition of a DASHPOTA element



Figure 71: Definition of a SPRINGA element

The two-node three-dimensional dashpot element is considered as a genuine three-dimensional element. Consequently, if it is connected to a 2D element with special restraints on the third direction (plane stress, plane strain or axisymmetric elements) the user has to take care that the third dimension does not induce rigid body motions in the dashpot nodes.

The dashpot element can only be used in linear dynamic calculations characterized by the *MODAL DYNAMIC keyword card.

6.2.31 Two-node 3-dimensional spring (SPRINGA)

This is a spring element defined between two nodes (Figure 71). The force needed in node 2 to extend the spring with original length L_0 to a final length L is given by:

$$\boldsymbol{F} = k(L - L_0)\boldsymbol{n}, \tag{9}$$

where k is the spring stiffness and $\boldsymbol{n}$ is a unit vector pointing from node 1 to node 2. The force in node 1 is $-\boldsymbol{F}$. This formula applies if the spring stiffness is constant. It is defined using the *SPRING keyword card. Alternatively, a nonlinear spring can be defined by providing a graph of the force versus the elongation. In calculations in which NLGEOM is active (nonlinear geometric calculations) the motion of nodes 1 and 2 induces a change of $\boldsymbol{n}$.

The two-node three-dimensional spring element is considered as a genuine three-dimensional element. Consequently, if it is connected to a 2D element with special restraints on the third direction (plane stress, plane strain or axisymmetric elements) the user has to take care that the third dimension does not induce rigid body motions in the spring nodes. An example of how to restrain the spring is given in test example spring4.

Note that a spring under compression, if not properly restrained, may change its direction by 180°, leading to unexpected results. Furthermore, for nonlinear springs, it does not make sense to extend the force-elongation curve to negative elongation values leL_0.

6.2.32 One-node coupling element (DCOUP3D)

This type is element is used to define the reference node of a distributing coupling constraint (cf. *DISTRIBUTING COUPLING). The node should not belong to any other element. The coordinates of this node are immaterial.

6.3 Beam General Section Types

A beam element is characterized by its cross section. If the cross section is rectangular (including square) or elliptical (including circular) the *BEAM SECTION card can be used. For all other section types the *BEAM GENERAL SECTION card has to be used. In that case, the beam element is internally expanded into a rectangular cross section (C3D20R-type element) and the actual section of the beam is simulated by an appropriate integration point scheme. A section type is characterized by a finite number of parameters, which must be entered immediately underneath the *BEAM GENERAL SECTION card. A new section type can be added by changing the following routines:

- beamgeneralsections.f (here, the one-letter abbreviation for the section has to be added. For instance, the pipe section is characterized by 'P'. Furthermore, the programmer must define the number of parameters needed to characterize the section).

- beamintscheme.f (here, the integration point scheme has to be defined)

- beamextscheme.f (here, the extrapolation of the integration point variables such as stresses or strains to the nodes of the expanded C3D20R element).

Right now, the following section types are available:

6.3.1 Pipe

The pipe section is circular and is characterized by its outer radius and its thickness (in that order). There are 8 integration points equally distributed along the circumference. In local coordinates, the radius at which the integration points are located is $\sqrt{(\xi^2+1)/2}$, where $\xi = r/R$, r being the inner radius and R the outer radius. The weight for each integration point is given by $\pi*(1-\xi^2)/8$ [12].

6.4 Fluid Section Types: Gases

A network element is characterized by a type of fluid section. It has to be specified on the *FLUID SECTION card unless the analysis is a pure thermomechanical calculation. For gases, the following types are available:

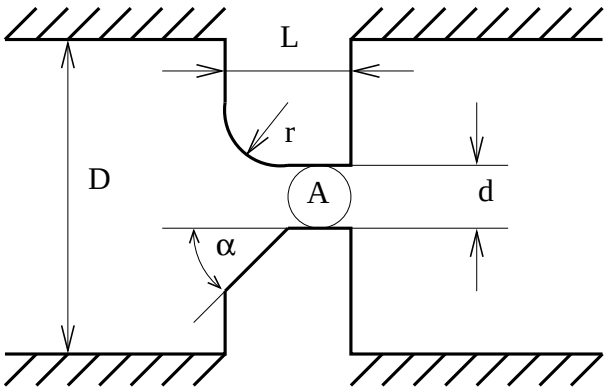


Figure 72: Geometry of the orifice fluid section

6.4.1 Orifice

The geometry of the orifice fluid section is shown in Figure 72. It is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION card):

- the cross section A.
- the orifice diameter d.
- the length L.
- the inlet corner radius r.
- the inlet corner angle α.
- the orifice-to-upstream pipe diameter ratio $\beta = d/D$.
- the rotational velocity v, if the orifice is part of a rotating structure.
- a reference network element.

Depending on the orifice geometry, an inlet corner radius or an inlet corner angle (chamfered inlet) should be selected. They are mutually exclusive. The corrections for a chamfered inlet are taken from [29].

The last constant, i.e. the number of a reference network element, is necessary in case a rotating structure is preceded by a network element which diverts the upstream air velocity from the axial direction (such as a preswirl nozzle). In that case, the rotational velocity of the orifice has to be corrected by the circumferential component of the velocity at the exit of the preceding element.

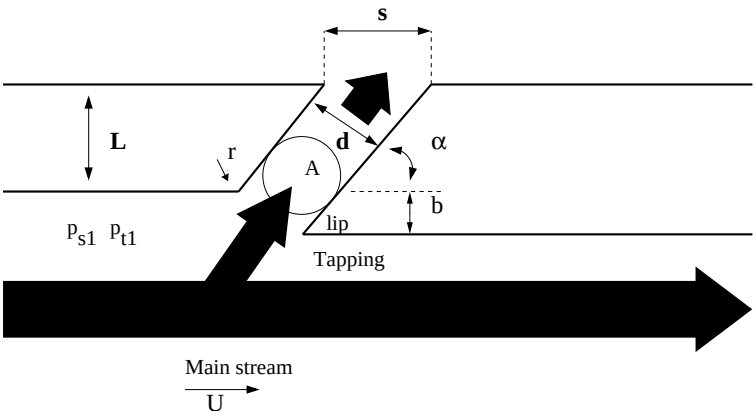


Figure 73: Geometry of the bleed tapping fluid section

The calculation of the discharge coefficient C_d can be performed according to different formulas. This is selected by the TYPE parameter:

- TYPE=ORIFICE_CD1 or just TYPE=ORIFICE: $C_d = 1$.
- TYPE=ORIFICE_MS_MS: Basis formula by McGreehan and Schotsch, rotational correction by McGreehan and Schotsch [46].
- TYPE=ORIFICE_PK_MS: Basis formula by Parker and Kercher [57], rotational correction by McGreehan and Schotsch [46].

Example files: linearnet, vortex1.

6.4.2 Bleed Tapping

A bleed tapping device is a special kind of orifice (Figure 73), used to divert part of the main stream flow. The geometry can be quite complicated and the discharge coefficient should be ideally determined by experiments on the actual device.

The discharge coefficients provided by CalculiX are merely a rough estimate and are based on [38]. For this purpose the bleed tapping device must be described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=BLEED TAPPING card):

- the cross section A.
- the ratio of the upstream static pressure to the upstream total pressure p_{s_1}/p_{t_1}.
- the number of a curve.

Right now, two curves are coded: curve number 1 corresponds to a tapping device with lip, curve number 2 to a tapping device without lip. More specific curves can be implemented by the user, the appropriate routine to do so is cd_bleedtapping.f. Alternatively, the usr can enter an own curve in the input deck listing $Y = C_d$ versus $X = (1 - p_{s_2}/p_{t_1})/(1 - p_{s_1}/p_{t_1})$. In that case the input reads

- the cross section A.
- the ratio of the upstream static pressure to the upstream total pressure p_{s_1}/p_{t_1}.
- not used
- X_1.
- Y_1.
- X_2.
- Y_2.
- ..

6.4.3 Preswirl Nozzle

A preswirl nozzle is a special kind of orifice (Figure 74), used to impart a tangential velocity to gas before it enters a rotating device. That way, the loss due to the difference in circumferential velocity between the air entering the rotating device and the rotating device itself can be decreased. In the Figure $\boldsymbol{v}_{rot}$ is the rotational velocity of the orifice the preswirl nozzle is serving, $\boldsymbol{v}_{abs}$ is the absolute velocity of the air leaving the preswirl nozzle and $\boldsymbol{v}_{rel}$ is its velocity as seen by an observer rotating with the orifice (the so-called relative velocity). The velocity entering the calculation of the discharge coefficient of the rotating orifice is the tangential component v of the velocity of the rotating device as seen by the air leaving the preswirl nozzle (which is $-\boldsymbol{v}_{rel}$). This velocity can be modified by a multiplicative factor k_ϕ.

The geometry of a preswirl nozzle can be quite complicated and the discharge coefficient should be ideally determined by experiments on the actual device.

The discharge coefficients provided by CalculiX are merely a rough estimate and are based on [38]. For this purpose the preswirl nozzle must be described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=PRESWIRL NOZZLE card):

- the cross section A.
- the angle with the engine axis at the exit of the nozzle.
- k_ϕ.

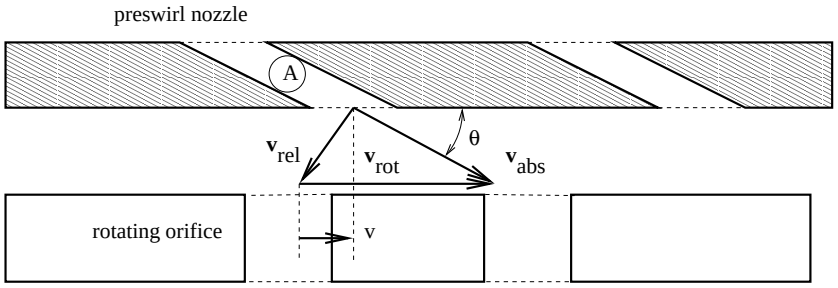


Figure 74: Geometry of the preswirl nozzle fluid section and the orifice it serves

- the number of a curve.

The angle at the exit of the nozzle is used to determine the circumferential velocity of the gas leaving the nozzle. This is stored for use in the (rotating) device following the nozzle. The curve number can be used to distinguish between several measured curves. Right now, only one curve is coded. More specific curves can be implemented by the user, the appropriate routine to do so is cd_preswirlnozzle.f. Alternatively, the usr can enter an own curve in the input deck listing $Y = C_d$ versus $X = p_{s_2}/p_{t_1}$. In that case the input reads

- the cross section A.
- the angle with the engine axis at the exit of the nozzle.
- k_ϕ.
- not used.
- not used.
- X_1.
- Y_1.
- X_2.
- Y_2.
- ..

Example files: moehring, vortex1, vortex2, vortex3.

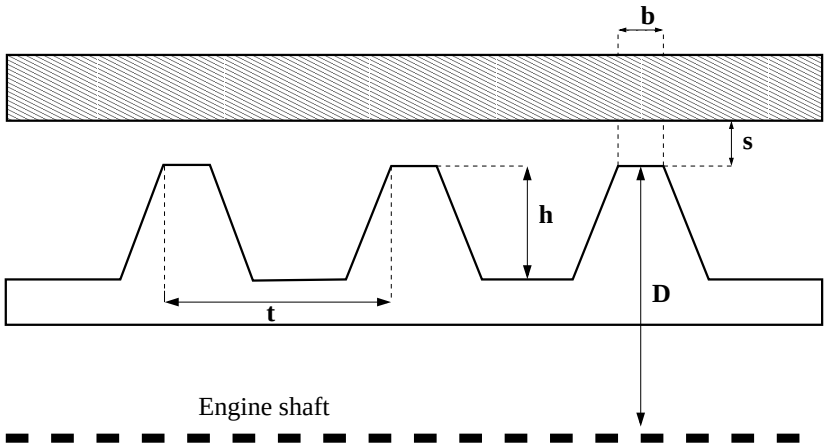


Figure 75: Geometry of straight labyrinth

6.4.4 Straight and Stepped Labyrinth

A labyrinth is used to prevent the gas from leaking through the space between a rotating and a static device and thus reducing the efficiency. The leaking air is trapped in the successive stages of a labyrinth. It can be straight (Figure 75) or stepped (Figure 76). A stepped labyrinth is used if the gas is compressed or expanded, leading to a decreasing and increasing diameter of the rotating device, respectively. In a stepped labyrinth the static device is usually covered by a honeycomb structure.

A LABYRINTH can be single (only one spike) or multiple (more than one spike). Only in the latter case the distinction between a straight and stepped labyrinth makes sense. Therefore, there are three kinds of labyrinths: single, straight or stepped.

The geometry of a labyrinth can be fixed or flexible during a calculation. For a fixed geometry the gap distance s is constant. For a flexible geometry this gap is defined as the distance between two nodes. These nodes have to be genuine structural nodes and should not belong to the fluid network. In a thermomechanical calculation this distance can vary during the computation. Whether the geometry is fixed or flexible is defined by the TYPE parameter.

The formula governing the flow through a labyrinth has been derived in [19] and for the discharge coefficients use was made of [46], [42], [14] and [82]. A fixed labyrinth is described by the following parameters (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=LABYRINTH SINGLE, TYPE=LABYRINTH STRAIGHT or TYPE=LABYRINTH STEPPED card):

- t: distance between two spikes
- s: gap between the top of the spike and the stator
- D: Diameter of the top of the spike

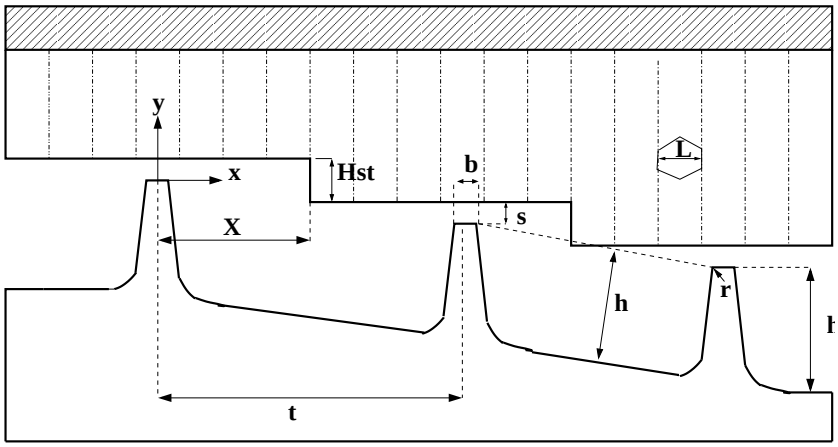


Figure 76: Geometry of stepped labyrinth

- n: number of spikes
- b: width of the top of the spike
- h: height of the spike measured from the bottom of the chamber
- L: width of a honeycomb cell
- r: edge radius of a spike
- X: distance between the spike and the next step
- Hst: height of the step

A flexible labyrinth is described by the following parameters (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=LABYRINTH FLEXIBLE SINGLE, TYPE=LABYRINTH FLEXIBLE STRAIGHT or TYPE=LABYRINTH FLEXIBLE STEPPED card):

- number of the first node defining the labyrinth gap
- number of the second node defining the labyrinth gap
- t: distance between two spikes
- D: Diameter of the top of the spike
- n: number of spikes
- b: width of the top of the spike
- h: height of the spike measured from the bottom of the chamber

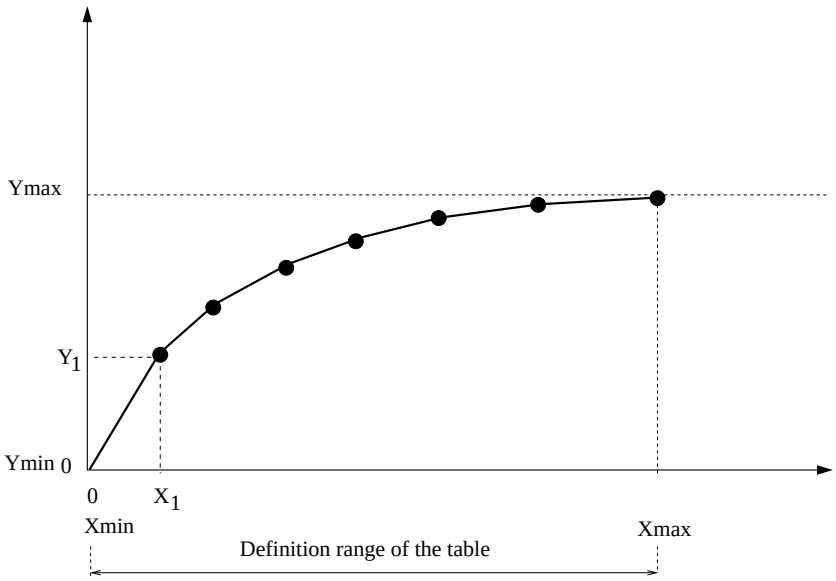


Figure 77: Characteristic Curve

- L: width of a honeycomb cell
- r: edge radius of a spike
- X: distance between the spike and the next step
- Hst: height of the step

Please look at the figures for the meaning of these parameters. Depending on the kind of labyrinth, not all parameters may be necessary.

Example files: labyrinthstepped, labyrinthstraight.

6.4.5 Characteristic

Sometimes a network element is described by its characteristic curve, expressing the reduced mass flow as a function of the pressure ratio (Figure 77). This allows the user to define new elements not already available.

The reduced flow is defined by

$$Y = \frac{\dot{m}\sqrt{\theta_1}}{p_1}, \tag{10}$$

where $\dot{m}$ is the mass flow, θ_1 is the upstream total temperature and p_1 is the upstream total pressure. The abscissa of the curve is defined by

$$X = \frac{p_1 - p_2}{p_1}, \tag{11}$$

where p_2 is the downstream total pressure. The characteristic curve is defined by the following parameters (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=CHARACTERISTIC card):

- scaling factor (default: 1)
- not used
- X_1
- Y_1
- X_2
- Y_2
- X_3
- Y_3
- X_4
- Y_4

Use more cards if more than three pairs are needed. No more than 9 pairs are allowed. In between the data points CalculiX performs an interpolation (solid line in Figure 77). In addition, the default point (0,0) is added as first point of the curve.

The scaling factor (first entry) is used to scale the ordinate values Y.

Example files: characteristic.

6.4.6 Carbon Seal

A carbon seal is used to prevent the gas from leaking through the space between a rotating and a static device and thus reducing the efficiency (Figure 78).

The formula governing the flow through a carbon seal has been derived in [61]. A carbon seal is described by the following parameters (to be specified in that order on the line beneath the *FLUID SECTION,TYPE=CARBON SEAL card):

- D: largest diameter of the gap
- s: size of the gap between rotor and carbon ring
- L: length of the carbon seal

Please look at the figure for the meaning of these parameters.

Example files: carbonseal.

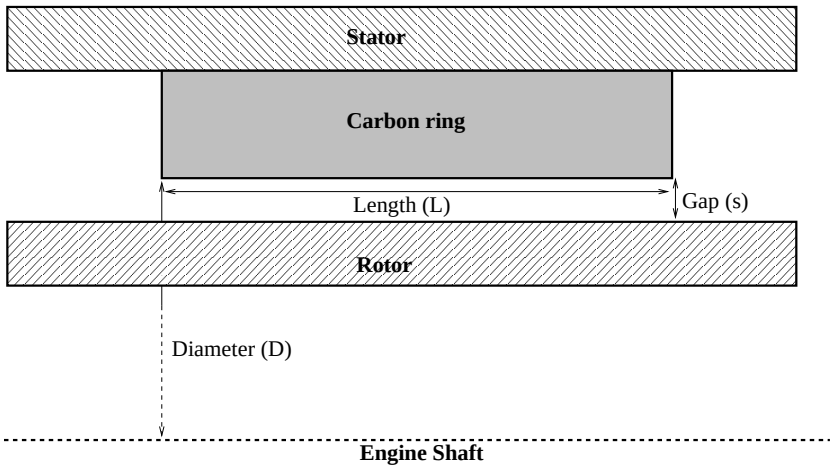


Figure 78: Geometry of a carbon seal

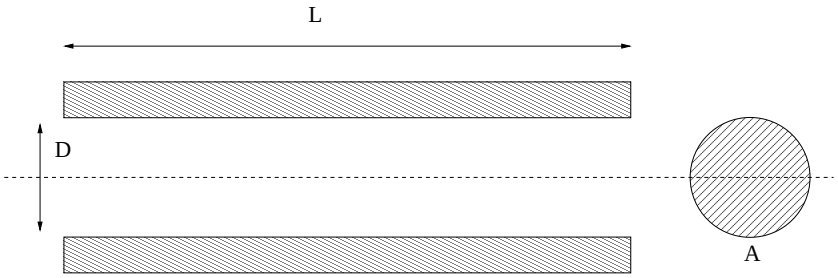


Figure 79: Geometry of the Gas Pipe element

6.4.7 Gas Pipe

The gas pipe element is a pipe element with constant cross section (Figure 79) It is allowed to rotate about an axis at a constant rotational speed. In that case the distance from the center point of the entrance r_{in} and of the exit r_{out} to the rotational axis have to be specified.

The friction parameter is determined as

$$f = \frac{64}{\mathrm{Re}} \tag{12}$$

for laminar flow ($\mathrm{Re} < 2000$) and

$$\frac{1}{\sqrt{f}} = -2.03 \log\left(\frac{2.51}{\mathrm{Re}\sqrt{f}} + \frac{k_s}{3.7D}\right). \tag{13}$$

for turbulent flow. Here, k_s is the diameter of the material grains at the surface of the pipe and Re is the Reynolds number defined by

$$\mathrm{Re} = \frac{UD}{\nu}, \tag{14}$$

where U is the liquid velocity and ν is the kinematic viscosity. A gas pipe is described by the following parameters (to be specified in that order on the line beneath the *FLUID SECTION,TYPE=GAS PIPE ADIABATIC or *FLUID SECTION,TYPE=GAS PIPE ISOTHERMAL card):

- A: cross section of the pipe
- D: hydraulic diameter of the pipe defined as 4 times the area divided by the perimeter
- L: length of the pipe
- k_s: grain diameter at the pipe surface
- form factor φ of the cross section
- oil mass flow in the pipe (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)
- not used
- entry radius r_{in}
- exit radius r_{out}
- rotational speed

The default gas pipe is adiabatic, i.e. there is no heat exchange with the pipe. Alternatively, the user may specify that the pipe element is isothermal. This means that the static temperature does not change within the pipe. In that case the energy equation in one of the two corner nodes of the element is replaced by a isothermal condition.

The form factor φ is only used to modify the friction expression for non-circular cross sections in the laminar regime as follows:

$$f = \varphi \frac{64}{\mathrm{Re}}. \tag{15}$$

Values for φ for several cross sections can be found in [13]. For a square cross section its value is 0.88, for a rectangle with a height to width ratio of 2 its value is 0.97.

Example files: gaspipe10, gaspipe8-cfd-massflow, gaspipe8-oil.

6.4.8 Gas Pipe (Fanno)

The gas pipe element of type Fanno is a pipe element with constant cross section (Figure 79), for which the Fanno formulae are applied [71].

It is described by the following parameters (to be specified in that order on the line beneath the *FLUID SECTION,TYPE=GAS PIPE FANNO ADIABATIC or *FLUID SECTION,TYPE=GAS PIPE FANNO ISOTHERMAL card):

- A: cross section of the pipe
- D: diameter of the pipe
- L: length of the pipe
- k_s: grain diameter at the pipe surface
- form factor φ
- oil mass flow in the pipe (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

The default gas pipe is adiabatic, i.e. there is no heat exchange with the pipe. Alternatively, the user may specify that the pipe element is isothermal. This means that the static temperature does not change within the pipe. In that case the energy equation in one of the two corner nodes of the element is replaced by a isothermal condition.

The form factor φ is only used to modify the friction expression for non-circular cross sections in the laminar regime as follows:

$$f = \varphi \frac{64}{\mathrm{Re}}. \tag{16}$$

Values for φ for several cross sections can be found in [13].

Example files: gaspipe-fanno10, gaspipe-fanno8-oil.

6.4.9 Restrictor, Long Orifice

Restrictors are discontinuous geometry changes in gas pipes. The pressure loss is characterized by [63]

$$\frac{p_{t_1}}{p_{t_2}} = \left(1 + \frac{\kappa - 1}{2} M_1^2\right)^{\zeta \frac{\kappa}{\kappa - 1}} \tag{17}$$

if ζ is defined with reference to the first section (e.g. for an enlargement, a bend or an exit) and

$$\frac{p_{t_1}}{p_{t_2}} = \left(1 + \frac{\kappa - 1}{2} M_2^2\right)^{\zeta \frac{\kappa}{\kappa - 1}} \tag{18}$$

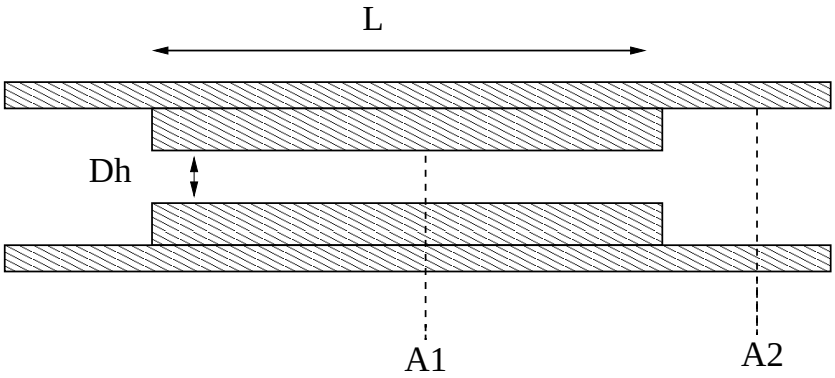


Figure 80: Geometry of a long orifice restrictor

if ζ refers to the second section (e.g. for a contraction or an entrance). p_{t_1} and M_1 are the total pressure and Mach number in section one, p_{t_2} and M_2 are the total pressure and Mach number in section two, ζ is the loss coefficient and κ the ratio of the heat capacity at constant pressure to the heat capacity at constant volume. These formulae apply to all restrictors if they are used for compressible fluids.

Restrictors can be applied to incompressible fluids as well, though, by specifying the parameter LIQUID on the *FLUID SECTION card. In that case the pressure losses amount to

$$\Delta_1^2 F = \zeta \frac{\dot{m}^2}{2g\rho^2 A_1^2} \tag{19}$$

and

$$\Delta_1^2 F = \zeta \frac{\dot{m}^2}{2g\rho^2 A_2^2}, \tag{20}$$

respectively.

A long orifice is a substantial reduction of the cross section of the pipe over a significant distance (Figure 80).

There are two types: TYPE=RESTRICTOR LONG ORIFICE IDELCHIK with loss coefficients according to [33] and TYPE=RESTRICTOR LONG ORIFICE LICHTAROWICZ with coefficients taken from [42]. In both cases the long orifice is described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=RESTRICTOR LONG ORIFICE IDELCHIK or TYPE=RESTRICTOR LONG ORIFICE LICHTAROWICZ card):

- reduced cross section A_1.
- full cross section A_2.

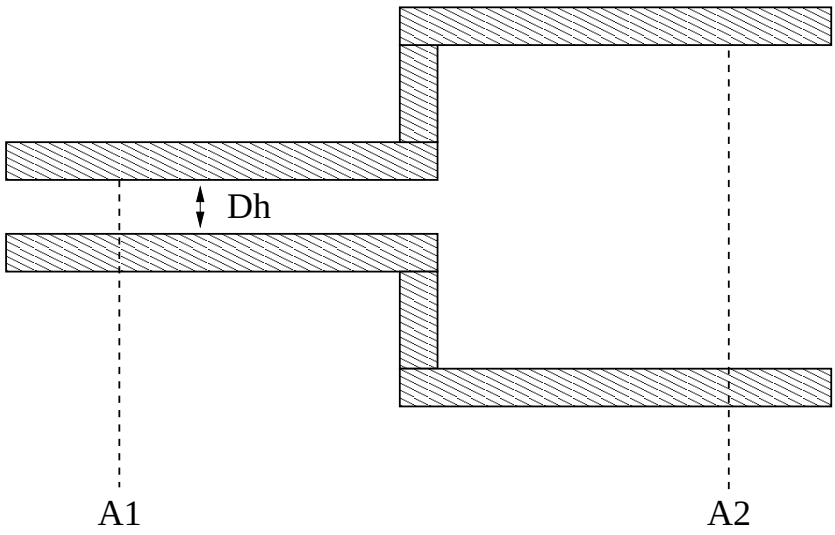


Figure 81: Geometry of an enlargement

- hydraulic diameter D_h defined by $D_h = 4A/P$ where P is the perimeter of the cross section.
- Length L of the orifice.
- oil mass flow in the restrictor (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

A restrictor of type long orifice MUST be preceded by a restrictor of type user with $\zeta = 0$. This accounts for the reduction of cross section from A_2 to A_1.

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

Example files: restrictor, restrictor-oil.

6.4.10 Restrictor, Enlargement

The geometry of an enlargement is shown in Figure 81. It is described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=RESTRICTOR ENLARGEMENT card):

- reduced cross section A_1.
- full cross section A_2.
- hydraulic diameter D_h defined by $D_h = 4A/P$ where P is the perimeter of the cross section.

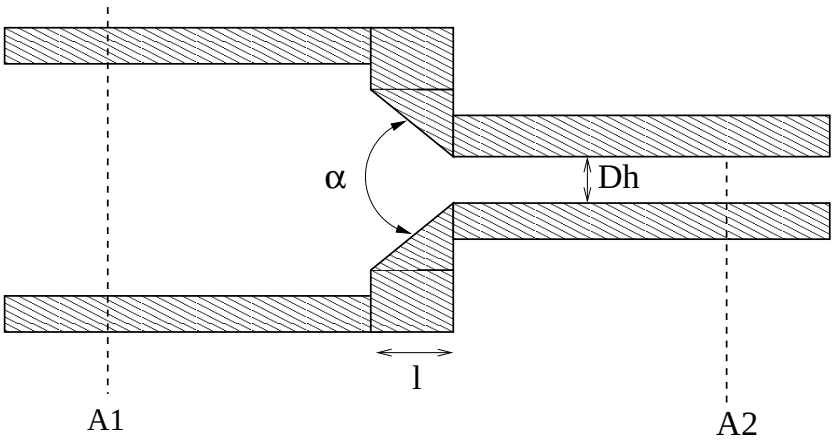


Figure 82: Geometry of a contraction

- oil mass flow in the restrictor (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

The loss coefficient for an enlargement is taken from [33].

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

Example files: piperestrictor, restrictor, restrictor-oil.

6.4.11 Restrictor, Contraction

The geometry of a contraction is shown in Figure 82. It is described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=RESTRICTOR CONTRACTION card):

- full cross section A_1.
- reduced cross section A_2.
- hydraulic diameter D_h defined by $D_h = 4A/P$ where P is the perimeter of the cross section.
- chamfer length L.
- chamfer angle α.
- oil mass flow in the restrictor (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

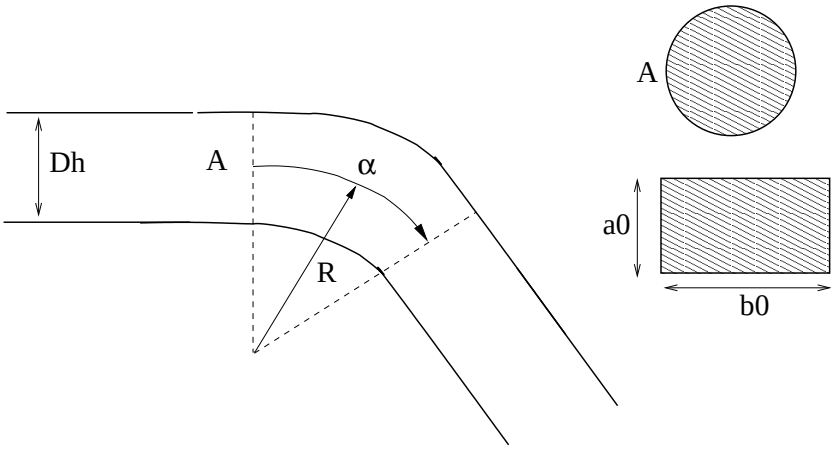


Figure 83: Geometry of a bend

The loss coefficient for a contraction is taken from [33].

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

Example files: piperestrictor, restrictor, restrictor-oil.

6.4.12 Restrictor, Bend

The geometry of a bend is shown in Figure 83. There are three types: TYPE = RESTRICTOR BEND IDEL CIRC, TYPE = RESTRICTOR BEND IDEL RECT, both with loss coefficients according to [33] and TYPE = RESTRICTOR BEND MILLER with coefficients taken from [52]. In the first and last type the bend is described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE = RESTRICTOR BEND IDEL CIRC or TYPE = RESTRICTOR BEND MILLER card):

- cross section before the bend A.
- cross section after the bend A.
- hydraulic diameter D_h.
- radius of the bend R.
- bend angle α.
- oil mass flow in the restrictor (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

They apply to circular cross sections. For rectangular cross sections the constants are as follows (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=RESTRICTOR BEND IDEL RECT card):

- cross section before the bend A.
- cross section after the bend A.
- hydraulic diameter D_h.
- radius of the bend R.
- bend angle α.
- height a_0.
- width b_0.
- oil mass flow in the restrictor (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

The loss coefficients are those published by Idelchik [33] and Miller [52].

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

Example files: restrictor, restrictor-oil.

6.4.13 Restrictor, Wall Orifice

The geometry of an wall orifice is shown in Figure 84. It is described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=RESTRICTOR WALL ORIFICE card):

- reduced cross section A.
- hydraulic diameter D_h defined by $D_h = 4A/P$ where P is the perimeter of the cross section.
- length L
- oil mass flow in the restrictor (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

The loss coefficient for a wall orifice is taken from [33].

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

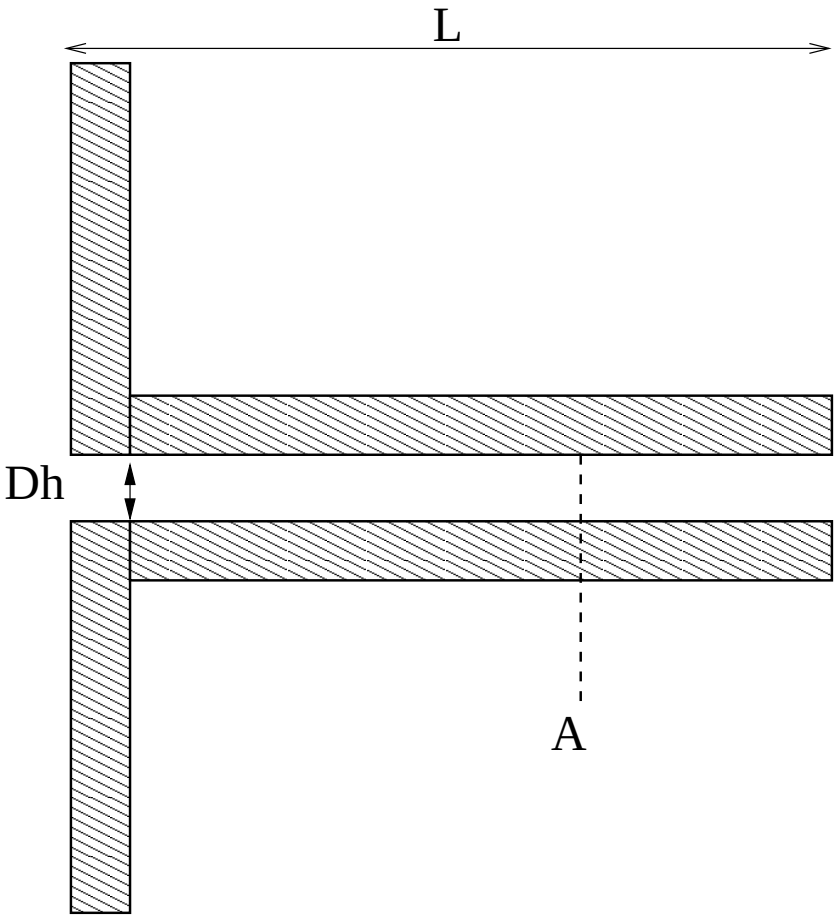


Figure 84: Geometry of a wall orifice

6.4.14 Restrictor, Entrance

An entrance element is used to model the entry from a large chamber into a gas pipe. For an entrance the value of ζ is 0.5. It is described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=RESTRICTOR ENTRANCE card):

- cross section of the entrance A.
- hydraulic diameter D_h defined by $D_h = 4A/P$ where P is the perimeter of the cross section.
- oil mass flow in the restrictor (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

6.4.15 Restrictor, Exit

An exit element is used to model the exit from a gas pipe into a large chamber. For an exit the value of ζ is 1. It is described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=RESTRICTOR EXIT card):

- cross section of the exit A.
- hydraulic diameter D_h defined by $D_h = 4A/P$ where P is the perimeter of the cross section.
- number of the upstream element; this element must be of type GAS PIPE
- oil mass flow in the restrictor (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

6.4.16 Restrictor, User

A user-defined restrictor is described by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=RESTRICTOR USER card):

- upstream cross section A_1.
- downstream cross section A_2.

- hydraulic diameter D_h defined by $D_h = 4A/P$ where A is the area of the smallest cross section and P is the perimeter of the smallest cross section.
- loss coefficient ζ.
- oil mass flow in the restrictor (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

Example files: restrictor, restrictor-oil.

6.4.17 Branch, Joint

In a joint the flow from two gas pipes is united and redirected through a third pipe. So in principal three network elements of type GAS PIPE have one node in common in a joint. The fluid elements of type BRANCH JOINT represent the extra energy loss due to the merging of the flows and have to be inserted on the incoming branches of the joint. This is represented schematically in Figure 85. The filled circles represent corner nodes of the fluid elements, the others are the midside nodes. For a joint to work properly the flow direction must be as indicated in Figure 85. If the solution of the equation system indicates that this is not the case appropriate measures must be taken. For instance, if the solution reveals that there is one inward flow and two outward flows, branch split elements must be selected.

Several types of geometry are available.

A branch joint of type GE [73], Figure 86, is quite general and allows arbitrary cross sections and angles (within reasonable limits). It is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=BRANCH JOINT GE card):

- label of the gas pipe element defined as branch 0.
- label of the gas pipe element defined as branch 1.
- label of the gas pipe element defined as branch 2.
- cross section A_0 of branch 0.
- cross section A_1 of branch 1.
- cross section A_2 of branch 2.
- angle α_1 (°).
- angle α_2 (°).

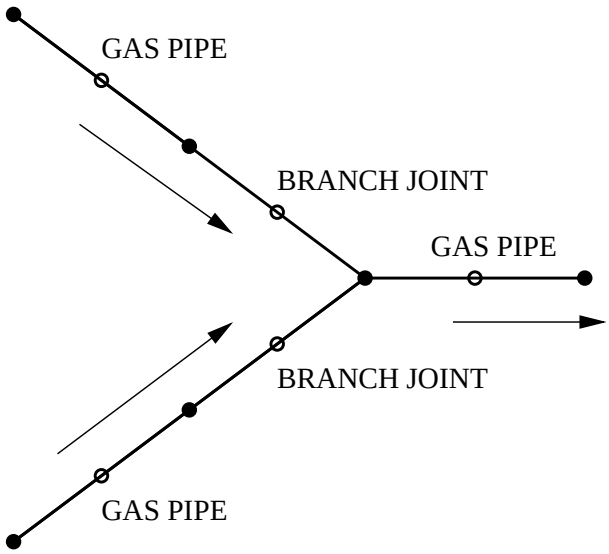


Figure 85: Element selection for a joint

- oil mass flow in branch 1 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)
- oil mass flow in branch 2 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

A branch joint of type Idelchik1, Figure 87, can be used if one of the incoming branches is continued in a straight way and does not change its cross section [33]. It is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=BRANCH JOINT IDELCHIK1 card):

- label of the gas pipe element defined as branch 0.
- label of the gas pipe element defined as branch 1.
- label of the gas pipe element defined as branch 2.
- cross section A_0 of branch 0.
- cross section $A_1 = A_0$ of branch 0.
- cross section A_2 of branch 2.
- angle $\alpha_1 = 0°$.
- angle α_2 (°).

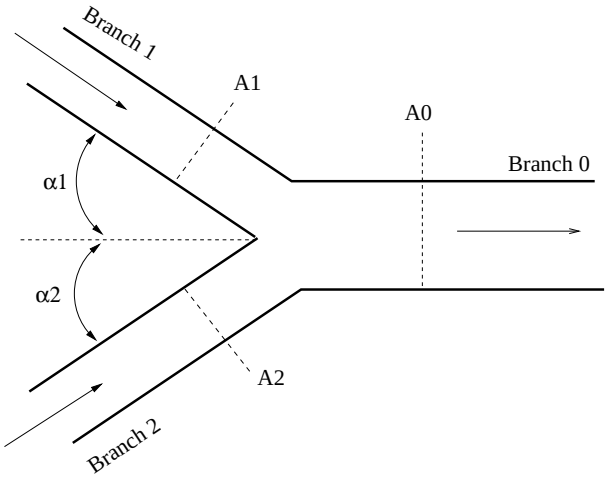


Figure 86: Geometry of a joint fluid section type GE

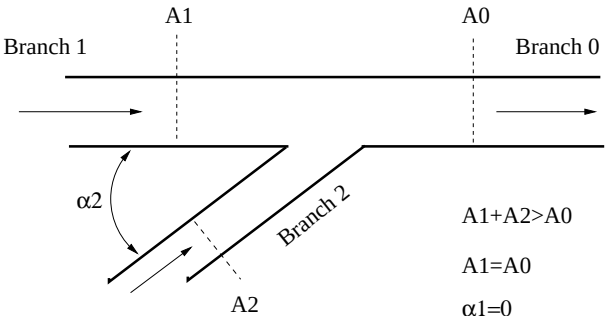


Figure 87: Geometry of a joint fluid section type Idelchik 1

- oil mass flow in branch 1 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)
- oil mass flow in branch 2 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

A branch joint of type Idelchik2, Figure 88, can be used if one of the incoming branches is continued in a straight way but may change its cross section [33]. It is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=BRANCH JOINT IDELCHIK2 card):

- label of the gas pipe element defined as branch 0.
- label of the gas pipe element defined as branch 1.
- label of the gas pipe element defined as branch 2.

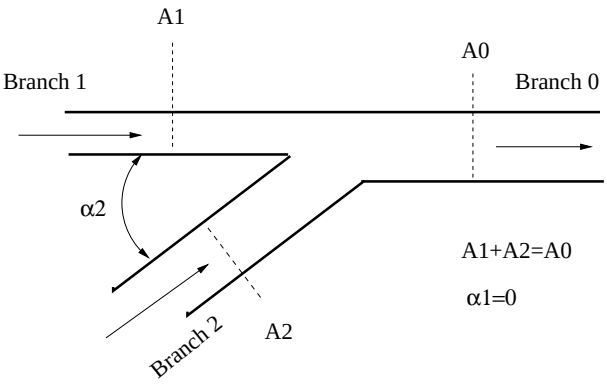


Figure 88: Geometry of a joint fluid section type Idelchik 2

- cross section A_0 of branch 0.
- cross section A_1 of branch 1.
- cross section A_2 of branch 2.
- angle $\alpha_1 = 0°$.
- angle α_2 (°).
- oil mass flow in branch 1 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)
- oil mass flow in branch 2 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

Example files: branchjoint1, branchjoint2, branchjoint3, branchjoint4.

6.4.18 Branch, Split

In a split the flow from a gas pipe is split and redirected through two other pipes. So in principal three network elements of type GAS PIPE have one node in common in a split. The fluid elements of type BRANCH SPLIT represent the extra energy loss due to the splitting of the flow and have to be inserted in the outward branches of the split. This is represented schematically in Figure 89. The filled circles represent corner nodes of the fluid elements, the others are the midside nodes. For a split to work properly the flow direction must be as indicated in Figure 89. If the solution of the equation system indicates that this is not the case appropriate measures must be taken. For instance, if the

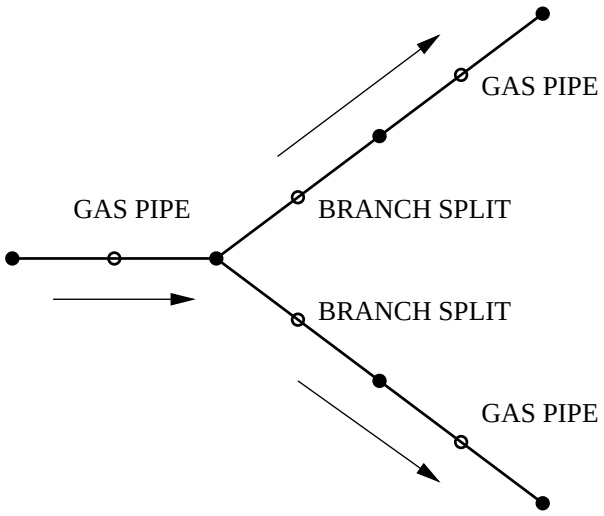


Figure 89: Element selection for a split

solution reveals that there are two inward flows and one outward flow, branch joint elements must be selected.

Several types of geometry are available.

A branch split of type GE [73], Figure 90, is quite general and allows arbitrary cross sections and angles (within reasonable limits). It is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=BRANCH SPLIT GE card):

- label of the gas pipe element defined as branch 0.
- label of the gas pipe element defined as branch 1.
- label of the gas pipe element defined as branch 2.
- cross section A_0 of branch 0.
- cross section A_1 of branch 1.
- cross section A_2 of branch 2.
- angle α_1 (°).
- angle α_2 (°).
- oil mass flow in branch 1 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)
- oil mass flow in branch 2 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

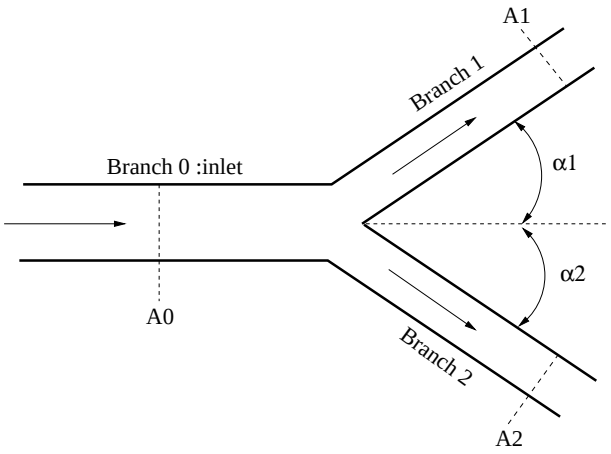


Figure 90: Geometry of a split fluid section type GE

A branch split of type Idelchik1, Figure 91, can be used if the incoming branch is continued in a straight way and does not change its cross section [33]. It is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=BRANCH SPLIT IDELCHIK1 card):

- label of the gas pipe element defined as branch 0.
- label of the gas pipe element defined as branch 1.
- label of the gas pipe element defined as branch 2.
- cross section A_0 of branch 0.
- cross section $A_1 = A_0$ of branch 0.
- cross section A_2 of branch 2.
- angle $\alpha_1 = 0°$.
- angle α_2 (°).
- hydraulic diameter D_{h0} of A_0.
- hydraulic diameter D_{h2} of A_2.
- oil mass flow in branch 1 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)
- oil mass flow in branch 2 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)

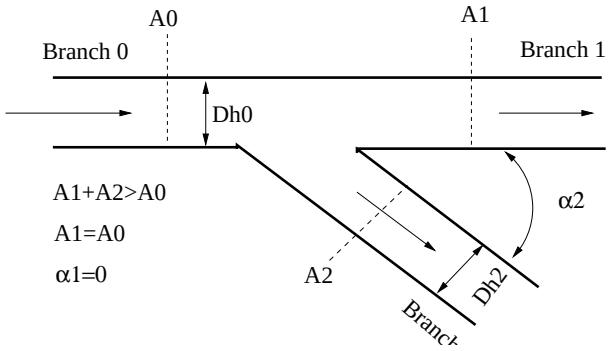


Figure 91: Geometry of a split fluid section type Idelchik 1

- ζ-correction factor k_1 for branch 1 ($\zeta_{eff} = k_1\zeta$). This allows to tune the ζ value with experimental evidence (default is 1).
- ζ-correction factor k_2 for branch 2 ($\zeta_{eff} = k_2\zeta$). This allows to tune the ζ value with experimental evidence (default is 1).

A branch split of type Idelchik2, Figure 92, is used if the outward branches make an angle of 90° with the incoming branch [33]. It is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=BRANCH SPLIT IDELCHIK2 card):

- label of the gas pipe element defined as branch 0.
- label of the gas pipe element defined as branch 1.
- label of the gas pipe element defined as branch 2.
- cross section A_0 of branch 0.
- cross section A_1 of branch 1.
- cross section A_2 of branch 2.
- angle $\alpha_1 = 90°$.
- angle $\alpha_2 = 90°$.
- oil mass flow in branch 1 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)
- oil mass flow in branch 2 (only if the OIL parameter is used to define the kind of oil in the *FLUID SECTION card)
- ζ-correction factor k_1 for branch 1 ($\zeta_{eff} = k_1\zeta$). This allows to tune the ζ value with experimental evidence (default is 1).

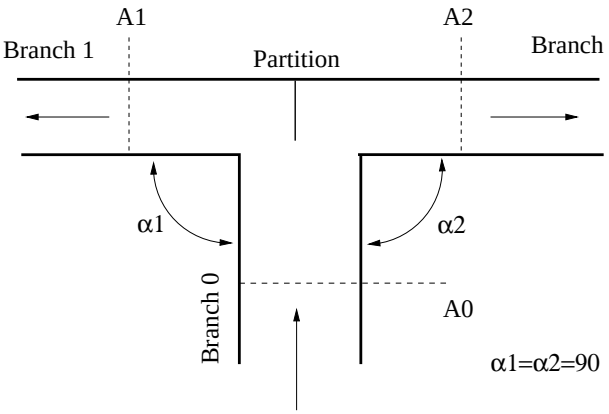


Figure 92: Geometry of a split fluid section type Idelchik 2

- ζ-correction factor k_2 for branch 2 ($\zeta_{eff} = k_2\zeta$). This allows to tune the ζ value with experimental evidence (default is 1).

By specifying the parameter LIQUID on the *FLUID SECTION card the loss is calculated for liquids. In the absence of this parameter, compressible losses are calculated.

Example files: branchsplit1, branchsplit2, branchsplit3.

6.4.19 Cross, Split

This is an element, in which a gas mass flow is split into three separate branches.(See Fig.93) It is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=CROSS SPLIT card):

- label of the element defined as branch 0.
- label of the element defined as branch 1.
- label of the element defined as branch 2.
- label of the element defined as branch 3.
- cross section A_0 of branch 0, whereas $A_1 = A_0$
- cross section A_2 of branch 2, whereas $A_3 = A_2$
- angle α_1.
- angle α_2.
- hydraulic diameter $d_{h0} = d_{h1}$

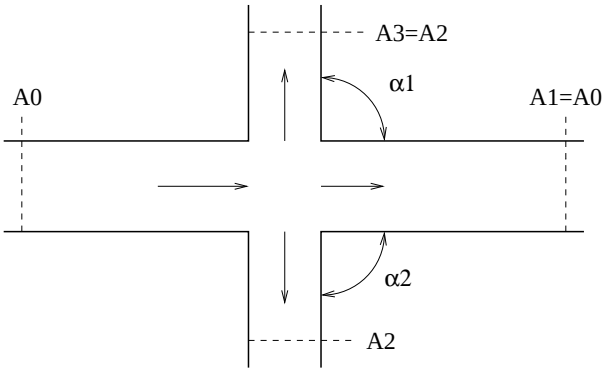


Figure 93: Geometry of a flow splitting cross

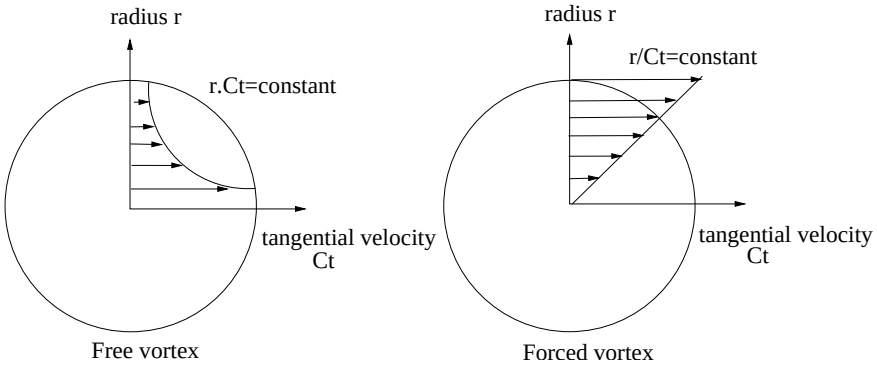


Figure 94: Forced vortex versus free vortex

- hydraulic diameter $d_{h2} = d_{h3}$
- ζ-correction factor k_1 for the main passage ($\zeta_{eff} = k_1\zeta$)
- ζ-correction factor k_2 for the branches ($\zeta_{eff} = k_2\zeta$)

6.4.20 Vortex

A vortex arises, when a gas flows along a rotating device. If the inertia of the gas is small and the device rotates at a high speed, the device will transfer part of its rotational energy to the gas. This is called a forced vortex. It is characterized by an increasing tangential velocity for increasing values of the radius, Figure 94.

Another case is represented by a gas exhibiting substantial swirl at a given radius and losing this swirl while flowing away from the axis. This is called a free vortex and is characterized by a hyperbolic decrease of the tangential

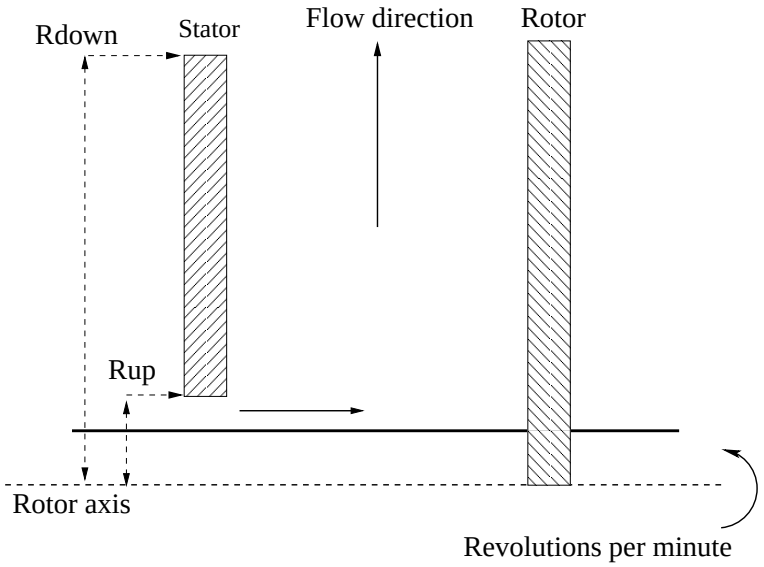


Figure 95: Geometry of a forced vortex

velocity, Figure 94. The initial swirl usually comes from a preceding rotational device.

The forced vortex, Figure 95 is geometrically characterized by its upstream and downstream radius. The direction of the flow can be centripetal or centrifugal, the element formulation works for both. The core swirl ratio K_r, which takes values between 0 and 1, denotes the degree the gas rotates with the rotational device. If $K_r = 0$ there is not transfer of rotational energy, if $K_r = 1$ the gas rotates with the device. The theoretical pressure ratio across a forced vertex satisfies

$$\left(\frac{p_o}{p_i}\right)_{theoretical} = \left[1 + \frac{(K_r U_i)^2}{2c_p T_i}\left(\left(\frac{R_o}{R_i}\right)^2 - 1\right)\right]^{\frac{\kappa}{\kappa-1}}, \tag{21}$$

where the index "i" stands for inside (smallest radius), "o" stands for outside (largest radius), p is the total pressure, T the total temperature and U the tangential velocity of the rotating device. It can be derived from the observation that the tangential velocity of the gas varies linear with the radius (Figure 94). Notice that the pressure at the outer radius always exceeds the pressure at the inner radius, no matter in which direction the flow occurs.

The pressure correction factor η allows for a correction to the theoretical pressure drop across the vortex and is defined by

$$\eta = \frac{\Delta p_{real}}{\Delta p_{theoretical}}. \tag{22}$$

Finally, the parameter $Tflag$ controls the temperature increase due to the vortex. In principal, the rotational energy transferred to the gas also leads to a temperature increase. If the user does not want to take that into account $Tflag = 0$ should be selected, else $Tflag = 1$ or $Tflag = -1$ should be specified, depending on whether the vortex is defined in the absolute coordinate system or in a relative system fixed to the rotating device, respectively. A relative coordinate system is active if the vortex element is at some point in the network preceded by an absolute-to-relative gas element and followed by a relative-to-absolute gas element. The calculated temperature increase is only correct for $K_r = 1$. Summarizing, a forced vortex element is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=VORTEX FORCED card):

- R_{down}: downstream radius
- R_{up}: upstream radius
- η: pressure correction factor
- K_r: core swirl ratio
- N: speed of the rotating device in rounds per minute
- $Tflag$

For the free vortex the value of the tangential velocity C_t of the gas at entrance is the most important parameter. It can be defined by specifying the number n of the preceding element, usually a preswirl nozzle or another vortex, imparting the tangential velocity. In that case the value N is not used. For centrifugal flow the value of the imparted tangential velocity $U_{theorical}$ can be further modified by the swirl loss factor K_1 defined by

$$K_1 = \frac{C_{t,real,i} - U_i}{C_{t,theoretical,i} - U_i}. \tag{23}$$

Alternatively, if the user specifies $n = 0$, the tangential velocity at entrance is taken from the rotational speed N of a device imparting the swirl to the gas. In that case K_1 and U_1 are not used. The theoretical pressure ratio across a free vertex satisfies

$$\left(\frac{p_o}{p_i}\right)_{theoretical} = \left[1 + \frac{C_{t,real,i}^2}{2c_pT_i}\left(1 - \left(\frac{R_i}{R_o}\right)^2\right)\right]^{\frac{\kappa}{\kappa-1}}, \tag{24}$$

where the index “i” stands for inside (smallest radius), “o” stands for outside (largest radius), “up” for upstream, p is the total pressure, T the total temperature and Ct the tangential velocity of the gas. It can be derived from the observation that the tangential velocity of the gas varies inversely proportional to the radius (Figure 94). Notice that the pressure at the outer radius always

exceeds the pressure at the inner radius, no matter in which direction the flow occurs.

Here too, the pressure can be corrected by a pressure correction factor η and a parameter $Tflag$ is introduced to control the way the temperature change is taken into account. However, it should be noted that for a free vortex the temperature does not change in the absolute system. Summarizing, a free vortex element is characterized by the following constants (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=VORTEX FREE card):

- R_{down}: downstream radius
- R_{up}: upstream radius
- η: pressure correction factor
- K_1: swirl loss factor
- U_{up}: tangential velocity of the rotating device at the upstream radius
- n: number of the gs element responsible for the swirl
- N: speed of the rotating device in rounds per minute
- $Tflag$

Example files: vortex1, vortex2, vortex3.

6.4.21 Möhring

A Möhring element is a vortex element for which the characteristics are determined by the integration of a nonlinear differential equation describing the physics of the problem [55]. It basically describes the flow in narrow gaps between a rotating and a static device and is more precise than the formulation of the forced and free vortex element. The geometry is shown in Figure 96 and consists of a minimum radius, a maximum radius, a value for the gap between stator and rotor and the shroud radius. It is complemented by the label of the upstream and downstream node, the rotating speed of the rotor and the value of the swirl at entrance. The user must choose the centrifugal or centripetal version of the Moehring element before start of the calculation, i.e. the user must decide beforehand in which direction the flow will move. If the calculation detects that the flow is reversed, an error message is issued.

The following constants must be entered (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=MOEHRING CENTRIFUGAL card or *FLUID SECTION, TYPE=MOEHRING CENTRIPETAL card):

- R_{min}: minimum radius
- R_{max}: maximum radius

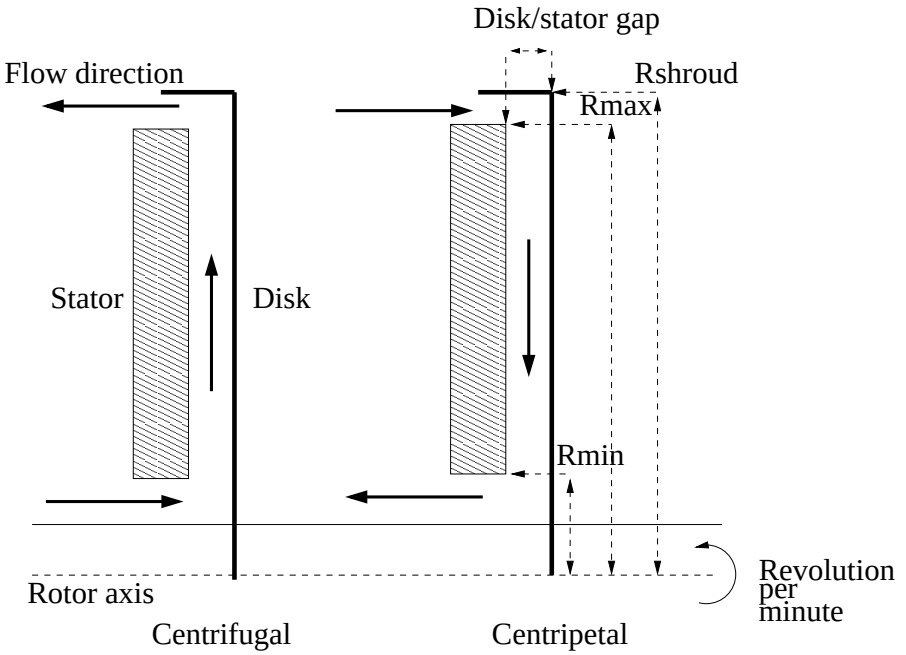


Figure 96: Geometry of the Möhring element

- d: disk/stator gap
- R_{shroud}: shroud radius
- upstream node label
- downstream node label
- N: speed of the rotor in rounds per minute
- tangential speed of the gas at entrance

Example files: moehring.

6.4.22 Change absolute/relative system

Sometimes it is more convenient to work in a relative system fixed to some rotating device, e.g. to model the flow through holes in a rotating disk. In order to facilitate this, two conversion elements were created: a relative-to-absolute element and an absolute-to-relative element. The transformation takes place at a given radius and the element has a physical length of zero. Input for this element is the circumferential velocity of the rotating device and the tangential gas velocity , both at the radius at which the transformation is to take place. The

gas velocity can be specified explicitly, or by referring to an element immediately preceding the transformation location and imparting a specific swirl to the gas. For an absolute-to-relative element the input is as follows (to be specified in that order on the line beneath the *FLUID SECTION, TYPE=ABSOLUTE TO RELATIVE card):

- U: circumferential velocity of the rotating device
- C_u: tangential gas velocity at the selected radius
- n: element immediately preceding the location of the transformation

C_u is taken if and only if $n = 0$. In all other cases the exit velocity of the element with label n is taken.

For an relative-to-absolute element the input is identical except that the type of the element is now RELATIVE TO ABSOLUTE.

Example files: moehring, vortex1, vortex2, vortex3.

6.4.23 In/Out

At locations where mass flow can enter or leave the network an element with node label 0 at the entry and exit, respectively, has to be specified. Its fluid section type for gas networks must be INOUT, to be specified on the *FLUID SECTION card. For this type there are no extra parameters.

6.5 Fluid Section Types: Liquids

A network element is characterized by a type of fluid section. It has to be specified on the *FLUID SECTION card unless the analysis is a pure thermo-mechanical calculation. For liquids the orifice (only for $C_d = 1$), restrictor, branch, and vortex fluid section types of gases can be used by specifying the parameter LIQUID on the *FLUID SECTION card. In addition, the following types are available as well (the coefficients for the head losses are taken from [10], unless specified otherwise):

6.5.1 Pipe, Manning

This is a straight pipe with constant section and head losses $\Delta_1^2 F$ defined by the Manning formula:

$$\Delta_1^2 F = \frac{n^2 \dot{m}^2 L}{\rho^2 A^2 \mathcal{R}^{4/3}}, \tag{25}$$

where n is the Manning coefficient (unit: time/length$^{1/3}$), $\dot{m}$ is the mass flux, L is the length of the pipe, ρ is the liquid density, A is the cross section of the pipe and $\mathcal{R}$ is the hydraulic radius defined by the area of the cross section divided by its circumference (for a circle the hydraulic radius is one fourth of

the diameter). The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE MANNING card:

- area of the cross section
- hydraulic radius of the cross section
- Manning coefficient n

The length of the pipe is determined from the coordinates of its end nodes. Typical values for n are $n = 0.013\text{s/m}^{1/3}$ for steel pipes and $n = 0.015\text{s/m}^{1/3}$ for smooth concrete pipes (these values are for water. Notice that, since the dynamic viscosity does not show up explicitly in the Manning formula, n may be a function of the viscosity).

By specifying the addition FLEXIBLE in the type label the user can create a flexible pipe. In that case the user specifies two nodes, the distance between them being the radius of the pipe. These nodes have to be genuine structural nodes and should not belong to the fluid network. The distance is calculated from the location of the nodes at the start of the calculation modified by any displacements affecting the nodes. Consequently, the use of the *COUPLED TEMPERATURE-DISPLACEMENT keyword allows for a coupling of the deformation of the pipe wall with the flow in the pipe. The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE MANNING FLEXIBLE card:

- node number 1
- node number 2
- Manning coefficient n

Example files: artery1, artery2, centheat1, centheat2, pipe, piperestrictor.

6.5.2 Pipe, White-Colebrook

This is a straight pipe with constant section and head losses $\Delta_1^2 F$ defined by the formula:

$$\Delta_1^2 F = \frac{f\dot{m}^2 L}{2g\rho^2 A^2 D}, \tag{26}$$

where f is the White-Colebrook coefficient (dimensionless), $\dot{m}$ is the mass flux, L is the length of the pipe, g is the gravity acceleration (9.81m/s^2), A is the cross section of the pipe and D is the diameter. The White-Colebrook coefficient satisfies the following implicit equation:

$$\frac{1}{\sqrt{f}} = -2.03 \log\left(\frac{2.51}{\text{Re}\sqrt{f}} + \frac{k_s}{3.7D}\right). \tag{27}$$

Here, k_s is the diameter of the material grains at the surface of the pipe and Re is the Reynolds number defined by

$$\mathrm{Re} = \frac{UD}{\nu}, \tag{28}$$

where U is the liquid velocity and ν is the kinematic viscosity. It satisfies $\nu = \mu/\rho$ where μ is the dynamic viscosity.

The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE WHITE-COLEBROOK card:

- area of the cross section
- hydraulic diameter of the cross section (4 times the area divided by the perimeter)
- length of the pipe element; if this number is nonpositive the length is calculated from the coordinates of the pipe's end nodes.
- the grain diameter k_s
- form factor φ of the cross section

The gravity acceleration must be specified by a gravity type *DLOAD card defined for the elements at stake. The material characteristics ρ and μ can be defined by a *DENSITY and *FLUID CONSTANTS card. Typical values for k_s are 0.25 mm for cast iron, 0.1 mm for welded steel, 1.2 mm for concrete, 0.006 mm for copper and 0.003 mm for glass.

The form factor φ is only used to modify the friction expression for non-circular cross sections in the laminar regime as follows:

$$f = \varphi \frac{64}{\mathrm{Re}}. \tag{29}$$

Values for φ for several cross sections can be found in [13]. For a square cross section its value is 0.88, for a rectangle with a height to width ratio of 2 its value is 0.97.

By specifying the addition FLEXIBLE in the type label the user can create a flexible pipe. In that case the user specifies two nodes, the distance between them being the radius of the pipe. These nodes have to be genuine structural nodes and should not belong to the fluid network. The distance is calculated from the location of the nodes at the start of the calculation modified by any displacements affecting the nodes. Consequently, the use of the *COUPLED TEMPERATURE-DISPLACEMENT keyword allows for a coupling of the deformation of the pipe wall with the flow in the pipe. The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE WHITE-COLEBROOK FLEXIBLE card:

- node number 1

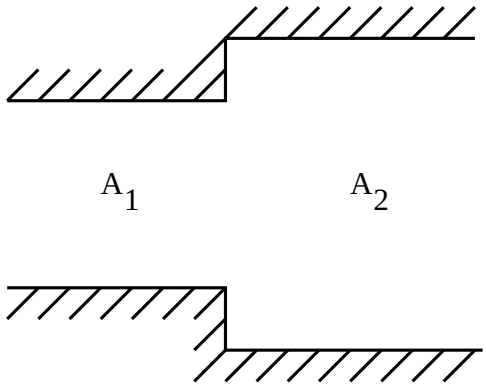


Figure 97: Sudden Enlargement

- node number 2
- length of the pipe element; if this number is nonpositive the length is calculated from the coordinates of the pipe's end nodes.
- the grain diameter k_s
- form factor φ of the cross section

Example files: pipe2.

6.5.3 Pipe, Sudden Enlargement

A sudden enlargement (Figure 97) is characterized by head losses $\Delta_1^2 F$ of the form:

$$\Delta_1^2 F = \zeta \frac{\dot{m}^2}{2g\rho^2 A_1^2}, \tag{30}$$

where ζ is a head loss coefficient depending on the ratio A_1/A_2, $\dot{m}$ is the mass flow, g is the gravity acceleration and ρ is the liquid density. A_1 and A_2 are the smaller and larger cross section, respectively. Notice that this formula is only valid for $\dot{m} \geq 0$. For a reverse mass flow, the formulas for a pipe contraction have to be taken. Values for ζ can be found in file "liquidpipe.f".

The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE ENLARGEMENT card:

- A_1

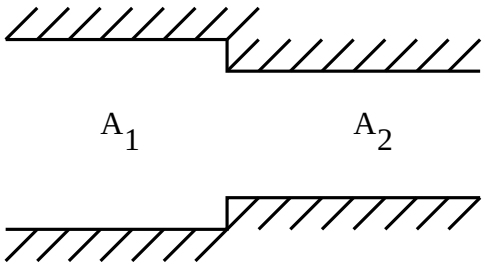


Figure 98: Sudden Contraction

- $A_2 (\geq A_1)$

The gravity acceleration must be specified by a gravity type *DLOAD card defined for the elements at stake. The material characteristic ρ can be defined by a *DENSITY card.

Example files: centheat1, pipe.

6.5.4 Pipe, Sudden Contraction

A sudden contraction (Figure 98) is characterized by head losses $\Delta_1^2 F$ of the form:

$$\Delta_1^2 F = \zeta \frac{\dot{m}^2}{2g\rho^2 A_2^2}, \tag{31}$$

where ζ is a head loss coefficient depending on the ratio A_2/A_1, $\dot{m}$ is the mass flow, g is the gravity acceleration and ρ is the liquid density. A_1 and A_2 are the larger and smaller cross section, respectively. Notice that this formula is only valid for $\dot{m} \geq 0$. For a reverse mass flow, the formulas for a pipe enlargement have to be taken. Values for ζ can be found in file "liquidpipe.f".

The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE CONTRACTION card:

- A_1
- $A_2 \quad (\leq A_1)$

The gravity acceleration must be specified by a gravity type *DLOAD card defined for the elements at stake. The material characteristic ρ can be defined by a *DENSITY card.

Example files: centheat1, pipe.

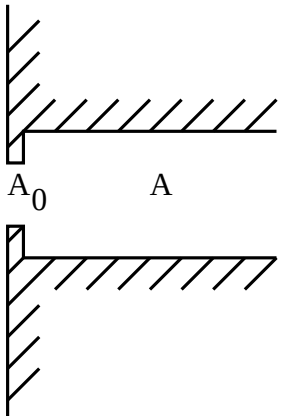


Figure 99: Entrance

6.5.5 Pipe, Entrance

A entrance (Figure 99) is characterized by head losses $\Delta_1^2 F$ of the form:

$$\Delta_1^2 F = \zeta \frac{\dot{m}^2}{2g\rho^2 A^2}, \tag{32}$$

where ζ is a head loss coefficient depending on the ratio A_0/A, $\dot{m}$ is the mass flow, g is the gravity acceleration and ρ is the liquid density. A_0 and A are the cross section of the entrance and of the pipe, respectively. Values for ζ can be found in file "liquidpipe.f".

The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE ENTRANCE card:

- A
- $A_0 \quad (\leq A)$

The gravity acceleration must be specified by a gravity type *DLOAD card defined for the elements at stake. The material characteristic ρ can be defined by a *DENSITY card.

Example files: pipe, piperestrictor.

6.5.6 Pipe, Diaphragm

A diaphragm (Figure 100) is characterized by head losses $\Delta_1^2 F$ of the form:

$$\Delta_1^2 F = \zeta \frac{\dot{m}^2}{2g\rho^2 A^2}, \tag{33}$$

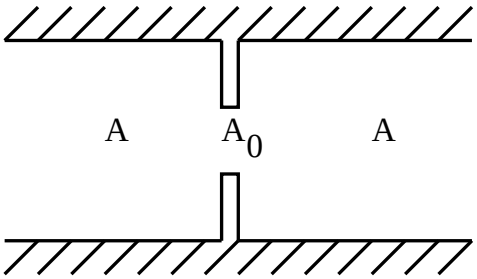


Figure 100: Diaphragm

where ζ is a head loss coefficient depending on the ratio A_0/A, $\dot{m}$ is the mass flow, g is the gravity acceleration and ρ is the liquid density. A_0 and A are the cross section of the diaphragm and of the pipe, respectively. Values for ζ can be found in file "liquidpipe.f".

The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE DIAPHRAGM card:

- A
- $A_0 \quad (\leq A)$

The gravity acceleration must be specified by a gravity type *DLOAD card defined for the elements at stake. The material characteristic ρ can be defined by a *DENSITY card.

6.5.7 Pipe, Bend

A bend (Figure 101) is characterized by head losses $\Delta_1^2 F$ of the form:

$$\Delta_1^2 F = \zeta \frac{\dot{m}^2}{2g\rho^2 A^2}, \tag{34}$$

where ζ is a head loss coefficient depending on the bend angle α and the ratio of the bend radius to the pipe diameter R/D, $\dot{m}$ is the mass flow, g is the gravity acceleration and ρ is the liquid density. A is the cross section of the pipe. Values for ζ can be found in file "liquidpipe.f".

The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE BEND card:

- A

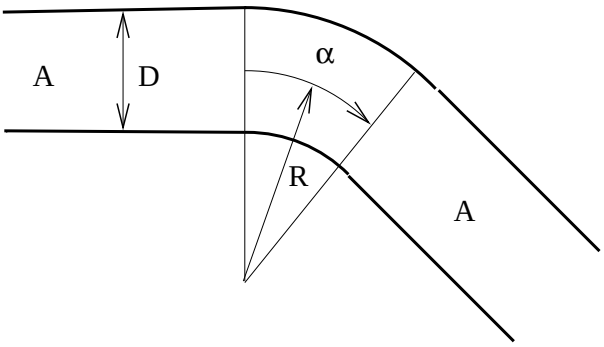


Figure 101: Bend

- $R/D \quad (\geq 1)$
- $\alpha \quad (\text{in } ^\circ)$
- $\xi \quad (0 \leq \xi \leq 1)$

ξ denotes the roughness of the pipe: $\xi = 0$ applies to an extremely smooth pipe surface, $\xi = 1$ to a very rough surface. The gravity acceleration must be specified by a gravity type *DLOAD card defined for the elements at stake. The material characteristic ρ can be defined by a *DENSITY card.

Example files: centheat1, pipe.

6.5.8 Pipe, Gate Valve

A gate valve (Figure 102) is characterized by head losses $\Delta_1^2 F$ of the form:

$$\Delta_1^2 F = \zeta \frac{\dot{m}^2}{2g\rho^2 A^2}, \tag{35}$$

where ζ is a head loss coefficient depending on the ratio $\alpha = x/D$, $\dot{m}$ is the mass flow, g is the gravity acceleration and ρ is the liquid density. A is the cross section of the pipe, x is a size for the remaining opening (Figure 102) and D is the diameter of the pipe. Values for ζ can be found in file "liquidpipe.f".

The following constants have to be specified on the line beneath the *FLUID SECTION, TYPE=PIPE GATE VALVE card:

- A

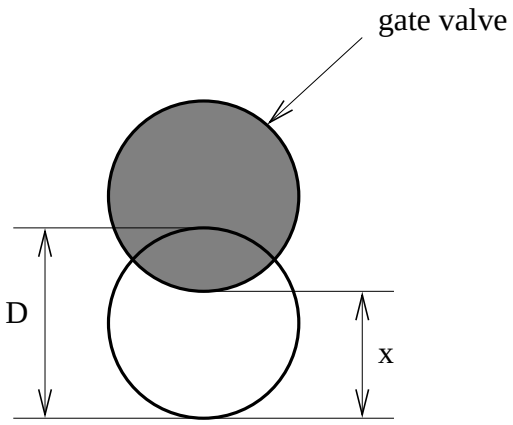


Figure 102: Gatevalve

- $\alpha \quad (0.125 \leq \alpha \leq 1)$

The gravity acceleration must be specified by a gravity type *DLOAD card defined for the elements at stake. The material characteristic ρ can be defined by a *DENSITY card.

For the gate valve the inverse problem can be solved too. If the user defines a value for $\alpha \leq 0$, α is being solved for. In that case the mass flow must be defined as boundary condition. Thus, the user can calculate the extent to which the valve must be closed to obtain a predefined mass flow. Test example pipe2.inp illustrates this feature.

Example files: pipe2, pipe, piperestrictor.

6.5.9 Pump

A pump is characterized by a total head increase versus total flow curve (Figure 103). The total head h is defined by:

$$h = z + \frac{p}{\rho g}, \tag{36}$$

where z is the vertical elevation, p is the pressure, ρ is the liquid density and g is the value of the earth acceleration. The total flow Q satisfies:

$$Q = \dot{m}/\rho, \tag{37}$$

where $\dot{m}$ is the mass flow. The pump characteristic can be defined underneath a *FLUID SECTION,TYPE=LIQUID PUMP by discrete data points on the curve. The data points should be given in increasing total flow order and

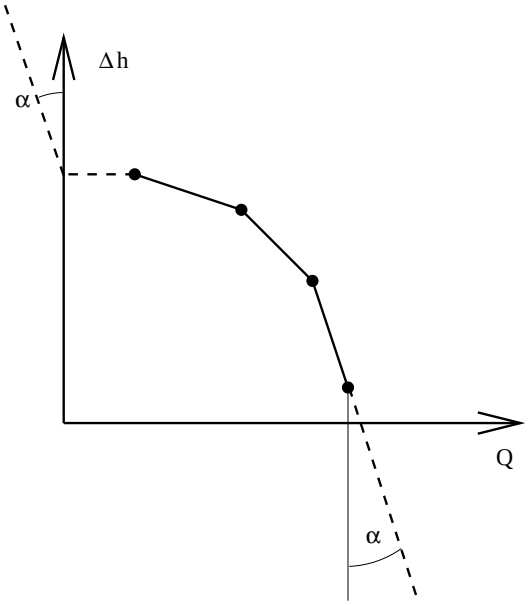


Figure 103: Pump Characteristic

the corresponding total head values must be decreasing. No more than 10 pairs are allowed. In between the data points CalculiX performs an interpolation (solid line in Figure 103). For flow values outside the defined range an extrapolation is performed, the form of which depends on the precise location of the flow (dashed lines in Figure 103). For positive flow values inferior to the lowest flow data point, the total head corresponding to this lowest flow data point is taken (horizontal dashed line). For negative flow values the total head sharply increases ($\alpha = 0.0001$) to simulate the zero-flow conditions of the pump in that region. For flow values exceeding the largest flow data point the total head decreases sharply with the same tangent α.

The gravity acceleration must be specified by a gravity type *DLOAD card defined for the elements at stake. The material characteristic ρ can be defined by a *DENSITY card.

Example files: centheat1.

6.5.10 In/Out

At locations where mass flow can enter or leave the network an element with node label 0 at the entry and exit, respectively, has to be specified. Its fluid section type for liquid pipe networks must be PIPE INOUT, to be specified on the *FLUID SECTION card. For this type there are no extra parameters.

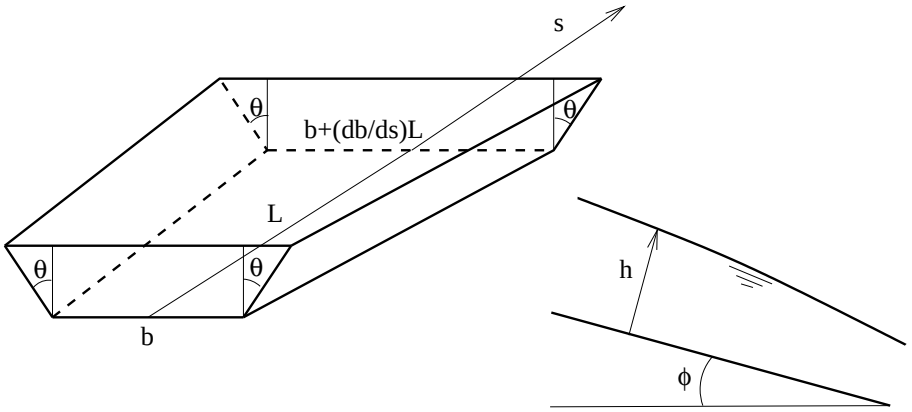


Figure 104: Channel geometry

6.6 Fluid Section Types: Open Channels

A network element is characterized by a type of fluid section. It has to be specified on the htmlref*FLUID SECTIONfluidsection card unless the analysis is a pure thermomechanical calculation (no calculation of pressure, mass flow or fluid depth). For an open channel network the boundary conditions for each branch are located upstream (frontwater flow) or downstream (backwater flow). These boundary conditions are made up of special elements, such as a sluice gate or a weir. Nearly all of these elements actually consist of pairs of elements, which reference each other. For instance, adjacent and downstream of the sluice gate element a sluice opening element has to be defined. The upstream element of such a pair has an additional degree of freedom attached to its middle node to accommodate the location of any hydraulic jump which might occur in the downstream channel branch. Therefore, all elements downstream of a pair of such boundary elements have to reference the upstream element of the pair. In our example, this is the sluice gate element. The friction in all elements is modeled by the White-Colebrook law, unless the parameter MANNING is specified on the *FLUID SECTION card. For details on these laws the reader is referred to Section 6.9.18.

6.6.1 Straight Channel

The straight channel is characterized by a trapezoid cross section, the bottom width of which can be defined to vary linearly. This is illustrated in Figure 104. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL STRAIGHT card:

- the width b
- the slope $S_0 = \sin\phi$ (if $S_0 < -1$ the slope is calculated from the coordinates of the end nodes belonging to the element)

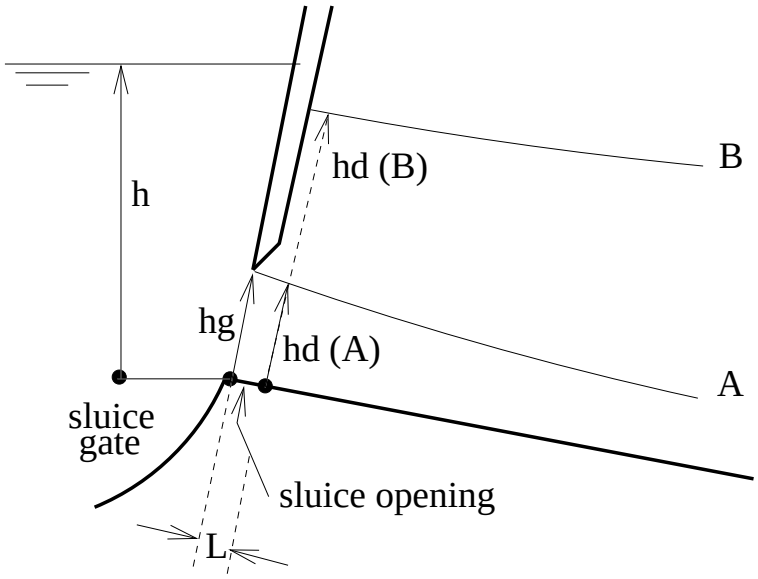


Figure 105: Sluice gate geometry

- the length L
- the trapezoid angle θ
- the grain diameter k_s for the White-Colebrook law or the Manning constant n for the Manning law (in the latter case the user has to specify the parameter MANNING on the *FLUID SECTION card)
- the number of the upstream reference element

Example files: channel1, chanson1.

6.6.2 Sluice Gate

The sluice gate is the upstream element of a pair of boundary elements simulating a sluice. The downstream element is the sluice opening. Both are illustrated in Figure 105. The interesting point is that the gate height h_g may be part of the backwater curve, but it does not have to. If the lower point of the gate is higher than the fluid surface, it will not be part of the backwater curve.

If the gate door touches the water and the water curve is a frontwater curve (curve A in Figure 105) the volumetric flow Q is given by

$$Q = bh_g\sqrt{2g(h - h_g\sqrt{1 - S_0^2})}, \tag{38}$$

if the gate door does not touch the water and the water curve is a frontwater curve the volumetric flow Q is given by

$$Q = bh_c\sqrt{2g(h - h_c\sqrt{1 - S_0^2})}, \tag{39}$$

where h_c is the critical depth. If the gate door touches the water and the water curve is a backwater curve (governed by downstream boundary conditions, curve B in Figure 105)) the volumetric flow is given by

$$Q = bh_g\sqrt{2g(h - h_d\sqrt{1 - S_0^2})}. \tag{40}$$

Finally, if the gate door does not touch the water and the water curve is a backwater curve the volumetric flow is given by

$$Q = bh_d\sqrt{2g(h - h_d\sqrt{1 - S_0^2})}. \tag{41}$$

The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL SLUICE GATE card:

- the width b
- the slope $S_0 = \sin\phi$ (if $S_0 < -1$ the slope is calculated from the coordinates of the end nodes belonging to the element)
- the height of the gate door h_g
- not used
- the number of the downstream sluice opening element
- the number of the upstream reference element, if any

The slope S_0 is used in case the gate door does not touch the water surface. The cross section of a sluice gate is supposed to be rectangular. Therefore, θ is lacking in its definition. Notice that a sluice gate can have upstream channel elements attached to it. In that case it is mandatory to specify an upstream reference element.

Example files: channel1, chanson1.

6.6.3 Sluice Opening

The sluice opening element is always adjacent to a sluice gate element on its upstream side. Both are illustrated in Figure 105. The sluice opening element has the gate door located at its upstream end node. Since the water depth in the downstream end node of this element should represent the depth just downstream of the gate door, the length of this element should be chosen to be particularly small. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL SLUICE OPENING card:

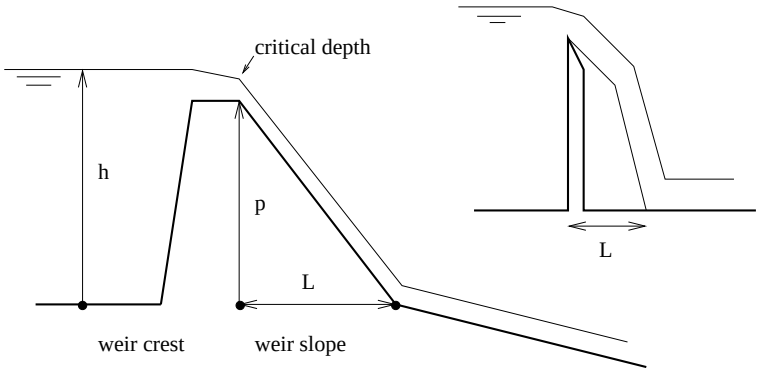


Figure 106: Weir geometry

- the width b
- the slope $S_0 = \sin\phi$ (if $S_0 < -1$ the slope is calculated from the coordinates of the end nodes belonging to the element)
- the length L (if $L \leq 0$ the length is calculated from the coordinates of the end nodes belonging to the element)
- the trapezoid angle θ
- the grain diameter k_s for the White-Colebrook law or the Manning constant n for the Manning law (in the latter case the user has to specify the parameter MANNING on the *FLUID SECTION card)
- the number of the upstream sluice gate element

The meaning of b, S_0, L and θ can be derived from Figure 104.

Example files: channel1, chanson1.

6.6.4 Weir Crest

The weir crest is the upstream element of a pair of boundary elements simulating a weir. The corresponding downstream element is the weir slope. Both are illustrated in Figure 106. The weir can occur in different forms such as broad-crested weirs (left picture in the Figure) and sharp-crested weirs (right picture in the Figure). The volumetric flow Q can be characterized by a law of the form

$$Q = Cb(h-p)^{3/2}, \tag{42}$$

where C is a constant. For instance, in the formula by Poleni $C = 2C_d\sqrt{2g}/3$, where C_d is coefficient smaller than 1 to be measured experimentally [11]. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL WEIR CREST card:

- the width b
- the height p
- the constant C
- not used
- the number of the downstream weir slope element
- the number of the upstream reference element, if any

The cross section of the weir is supposed to be rectangular. This is important, since a different form leads to a different exponent in Equation 42. Notice that a weir can have upstream channel elements attached to it. In that case it is mandatory to specify an upstream reference element.

Example files: channel7.

6.6.5 Weir slope

The weir slope is the downstream element of the boundary element pair defining a weir. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL WEIR SLOPE card:

- the width b
- the slope $S_0 = \sin\phi$ (if $S_0 < -1$ the slope is calculated from the coordinates of the end nodes belonging to the element)
- the length L (if $L \leq 0$ the length is calculated from the coordinates of the end nodes belonging to the element)
- the trapezoid angle θ
- the grain diameter k_s for the White-Colebrook law or the Manning constant n for the Manning law (in the latter case the user has to specify the parameter MANNING on the *FLUID SECTION card)
- the number of the upstream weir crest element

The meaning of b and θ can be derived from Figure 104. The value of S_0 is used to determine the critical depth on the crest. Moreover, it is used in the Bresse equation in case the flow is determined by the downstream conditions (inundated crest). It should simulate the mean slope in the absence of the weir. The length L of the weir is shown in Figure 106.

Example files: channel7.

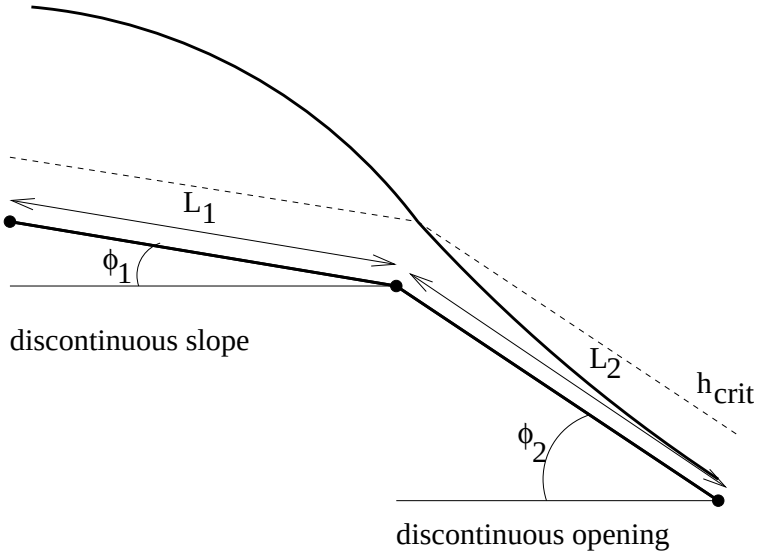


Figure 107: Geometry of a discontinuous slope

6.6.6 Discontinuous Slope

The discontinuous slope is the upstream element of a pair of boundary elements simulating a change in slope. The corresponding downstream element is the discontinuous opening. Both are illustrated in Figure 107. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL DISCONTINUOUS SLOPE card:

- the width b
- $S_0 = \sin(\phi_1)$ (Figure 107; if $S_0 < -1$ the slope is calculated from the coordinates of the end nodes belonging to the element)
- the length L_1 (Figure 107; if $L_1 \leq 0$ the length is calculated from the coordinates of the end nodes belonging to the element)
- the trapezoid angle θ
- the grain diameter k_s for the White-Colebrook law or the Manning constant n for the Manning law (in the latter case the user has to specify the parameter MANNING on the *FLUID SECTION card)
- the number of the upstream reference element
- not used
- the number of the downstream discontinuous opening element
- not used

The length L_1 is typically small compared to the length of the adjacent channel branches. Since storage for 9 items is provided and only 8 entries are allowed per line, an extra blank line has to be provided for the ninth dummy item.

Notice that a discontinuous slope element generally has upstream channel elements attached to it. Therefore, it is always mandatory to specify an upstream reference element.

Example files: channel6.

6.6.7 Discontinuous Opening

The discontinuous opening is the downstream element of the boundary element pair defining a change in channel slope. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL DISCONTINUOUS OPENING card:

- the width b
- $S_0 = \sin(\phi_2)$ (Figure 107; if $S_0 < -1$ the slope is calculated from the coordinates of the end nodes belonging to the element)
- the length L_2 (Figure 107; if $L_2 \leq 0$ the length is calculated from the coordinates of the end nodes belonging to the element)
- the trapezoid angle θ
- the grain diameter k_s for the White-Colebrook law or the Manning constant n for the Manning law (in the latter case the user has to specify the parameter MANNING on the *FLUID SECTION card)
- the number of the upstream discontinuous slope element.

The length L_2 is typically small compared to the length of the adjacent channel branches.

Example files: channel6.

6.6.8 Reservoir

A reservoir is a downstream boundary condition. The reservoir element represents the part of the channel immediately upstream of the (usually vast) reservoir. Since the backwater curve may change substantially in the neighborhood of the reservoir it is advisable to choose the length of the reservoir element to be small compared to the length of the channel branch it is part of. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL RESERVOIR card:

- the width b

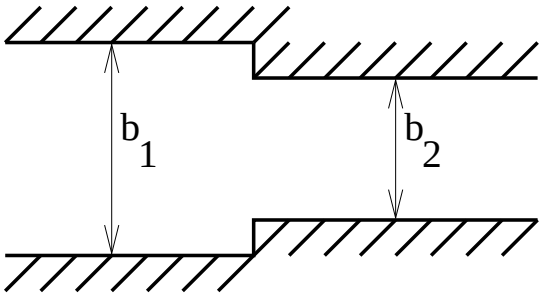


Figure 108: Geometry of a contraction

- the slope $S_0 = \sin\phi$ (if $S_0 < -1$ the slope is calculated from the coordinates of the end nodes belonging to the element)
- the length L (if $L \leq 0$ the length is calculated from the coordinates of the end nodes belonging to the element)
- the trapezoid angle θ
- the grain diameter k_s for the White-Colebrook law or the Manning constant n for the Manning law (in the latter case the user has to specify the parameter MANNING on the *FLUID SECTION card)
- the number of the upstream reference element, i.e. the first element of the boundary pair upstream of the channel branch connected to the reservoir.

The water depth in the downstream node of a reservoir element must be defined by the user by means of a *BOUNDARY card (degree of freedom 2).

Example files: channel1, chanson1.

6.6.9 Contraction

The geometry of a contraction is shown in Figure 108 (view from above). Although a contraction is really a discontinuity, a small fictitious length an a slope have to be assigned. For the slope one can take the mean values of the slopes of the adjacent channels. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL CONTRACTION card:

- the upstream width b_1

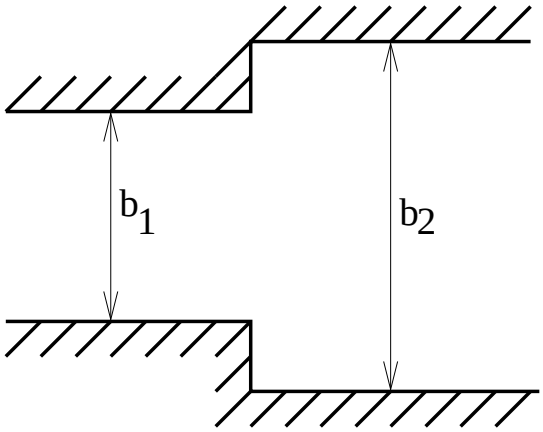


Figure 109: Geometry of an enlargement

- the slope S_0 (if $S_0 < -1$ zero is taken)
- the length L (if $L \leq 0$ the length is calculated from the coordinates of the end nodes belonging to the element)
- the downstream width $b_2 \leq b_1$

Example files: channel9, channel11.

6.6.10 Enlargement

The geometry of an enlargement is shown in Figure 109 (view from above). Although an enlargement is really a discontinuity, a small fictitious length an a slope have to be assigned. For the slope one can take the mean values of the slopes of the adjacent channels. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL ENLARGEMENT card:

- the upstream width b_1
- the slope S_0 (if $S_0 < -1$ zero is taken)
- the length L (if $L \leq 0$ the length is calculated from the coordinates of the end nodes belonging to the element)
- the downstream width $b_2 \geq b_1$

Example files: channel9, channel11.

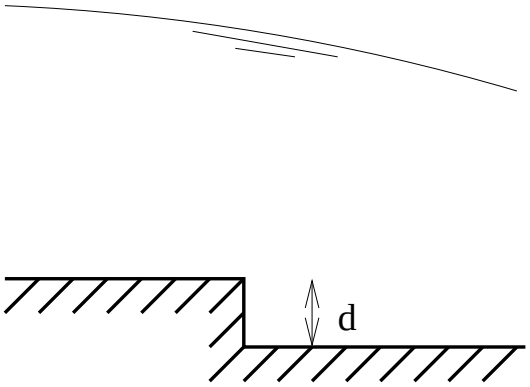


Figure 110: Geometry of a drop

6.6.11 Drop

The geometry of a drop is shown in Figure 110. Although a drop is really a discontinuity, a small fictitious length an a slope have to be assigned. For the slope one can take the mean values of the slopes of the adjacent channels. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL DROP card:

- the width b
- the slope S_0 (if $S_0 < -1$ zero is taken)
- the length L (if $L \leq 0$ the length is calculated from the coordinates of the end nodes belonging to the element)
- the drop size d

Example files: channel10, channel12.

6.6.12 Step

The geometry of a step is the inverse of the drop geometry. Although a step is really a discontinuity, a small fictitious length an a slope have to be assigned. For the slope one can take the mean values of the slopes of the adjacent channels. The following constants have to be specified on the line beneath the *FLUID SECTION,TYPE=CHANNEL STEP card:

- the width b
- the slope S_0 (if $S_0 < -1$ zero is taken)

- the length L (if $L \leq 0$ the length is calculated from the coordinates of the end nodes belonging to the element)
- the step size d

Example files: channel10, channel12.

6.6.13 In/Out

At locations where mass flow can enter or leave the network an element with node label 0 at the entry and exit, respectively, has to be specified. Its fluid section type for liquid channel networks must be CHANNEL INOUT, to be specified on the *FLUID SECTION card. For this type there are no extra parameters.

6.7 Boundary conditions

6.7.1 Single point constraints (SPC)

In a single point constraint one or more degrees of freedom are fixed for a given node. The prescribed value can be zero or nonzero. Nonzero SPC's cannot be defined outside a step. Zero SPC's can be defined inside or outside a step. SPC's are defined with the keyword *BOUNDARY. The mechanical degrees of freedom are labeld 1 through 6 (1 = translation in x, 2 = translation in y, 3 = translation in z, 4 = rotation about x, 5 = rotation about y, 6 = rotation about z), the thermal degree of freedom is labeled 11. Rotational degrees of freedom can be applied to beam and shell elements only.

6.7.2 Multiple point constraints (MPC)

Multiple point constraints establish a relationship between degrees of freedom in one or more nodes. In this section, only linear relationships are considered (for nonlinear relations look at the keyword *MPC and section 8.7).They must be defined with the keyword *EQUATION before the first step. An inhomogeneous linear relationship can be defined by assigning the inhomogeneous term to one of the degrees of freedom (DOF) of a dummy node (using a SPC) and including this DOF in the MPC, thus homogenizing it. The numbering of the DOF's is the same as for SPC's (cf previous section). It is not allowed to mix thermal and mechanical degrees of freedom within one and the same MPC.

6.7.3 Mathematical description of a knot

The mathematical description of a knot was inspired by the polar decomposition theorem stating that the deformed state $d\boldsymbol{x}$ of an infinitesimal vector $d\boldsymbol{X}$ in a continuum can be decomposed into a stretch followed by a rotation [18],[20]:

$$d\boldsymbol{x} = \boldsymbol{F} \cdot d\boldsymbol{X} = \boldsymbol{R} \cdot \boldsymbol{U} \cdot d\boldsymbol{X}, \tag{43}$$

where $\boldsymbol{F}$ is the deformation gradient, $\boldsymbol{R}$ is the rotation tensor and $\boldsymbol{U}$ is the right stretch tensor. Applying this to a finite vector extending from the center of gravity of a knot $\boldsymbol{q}$ to any expanded node $\boldsymbol{p_i}$ yields

$$(\boldsymbol{p_i} + \boldsymbol{u_i}) - (\boldsymbol{q} + \boldsymbol{w}) = \boldsymbol{R} \cdot \boldsymbol{U} \cdot (\boldsymbol{p_i} - \boldsymbol{q}), \tag{44}$$

where $\boldsymbol{u_i}$ and $\boldsymbol{w}$ are the deformation of the node and the deformation of the center of gravity, respectively. This can be rewritten as

$$\boldsymbol{u_i} = \boldsymbol{w} + (\boldsymbol{R} \cdot \boldsymbol{U} - \boldsymbol{I}) \cdot (\boldsymbol{p_i} - \boldsymbol{q}), \tag{45}$$

showing that the deformation of a node belonging to a knot can be decomposed in a translation of the knot's center of gravity followed by a stretch and a rotation of the connecting vector. Although this vector has finite dimensions, its size is usually small compared to the overall element length since it corresponds to the thickness of the shells or beams. In three dimensions $\boldsymbol{U}$ corresponds to a symmetric 3 x 3 matrix (6 degrees of freedom) and $\boldsymbol{R}$ to an orthogonal 3 x 3 matrix (3 degrees of freedom) yielding a total of 9 degrees of freedom. Notice that the stretch tensor can be written as a function of its principal values λ_i and principal directions $\boldsymbol{N^i}$ as follows:

$$\boldsymbol{U} = \sum_i \lambda_i \boldsymbol{N^i} \otimes \boldsymbol{N^i}. \tag{46}$$

Beam knot The expansion of a single beam node leads to a planar set of nodes. Therefore, the stretch of a knot based on this expansion is reduced to the stretch along the two principal directions in that plane. The stretch in the direction of the beam axis is not relevant. Let us assume that $\boldsymbol{T_1}$ is a unit vector tangent to the local beam axis and $\boldsymbol{E_1}, \boldsymbol{E_2}$ are two unit vectors in the expansion plane such that $\boldsymbol{E_1} \cdot \boldsymbol{E_2} = 0$ and $\boldsymbol{E_1} \times \boldsymbol{E_2} = \boldsymbol{T_1}$. Then, the stretch in the plane can be characterized by vectors $\boldsymbol{T_2}$ and $\boldsymbol{T_3}$ along its principal directions:

$$\boldsymbol{T_2} = \xi(\boldsymbol{E_1} \cos\varphi + \boldsymbol{E_2} \sin\varphi) \tag{47}$$

$$\boldsymbol{T_3} = \eta(-\boldsymbol{E_1} \sin\varphi + \boldsymbol{E_2} \cos\varphi) \tag{48}$$

leading to three stretch degrees of freedom φ, ξ and η. φ is the angle $\boldsymbol{T_2}$ makes with $\boldsymbol{E_1}$, ξ is the stretch along $\boldsymbol{T_2}$ and η is the stretch along $\boldsymbol{T_3}$. The right stretch tensor $\boldsymbol{U}$ can now be written as:

$$\begin{aligned}\boldsymbol{U} &= \boldsymbol{T_1} \otimes \boldsymbol{T_1} + \boldsymbol{T_2} \otimes \boldsymbol{T_2} + \boldsymbol{T_3} \otimes \boldsymbol{T_3} \\ &= \boldsymbol{T_1} \otimes \boldsymbol{T_1} + (\xi^2 \cos^2\varphi + \eta^2 \sin^2\varphi)\boldsymbol{E_1} \otimes \boldsymbol{E_1} + (\xi^2 \sin^2\varphi + \eta^2 \cos^2\varphi)\boldsymbol{E_2} \otimes \boldsymbol{E_2} \\ &+ (\xi^2 - \eta^2)\cos\varphi \sin\varphi(\boldsymbol{E_1} \otimes \boldsymbol{E_2} + \boldsymbol{E_2} \otimes \boldsymbol{E_1}).\end{aligned} \tag{49}$$

The rotation vector reads in component notation

$$R_{ij} = \delta_{ij} \cos\theta + \sin\theta e_{ikj} n_k + (1 - \cos\theta) n_i n_j. \tag{50}$$

Here, $\boldsymbol{\theta}$ is a vector along the rotation axis satisfying $\boldsymbol{\theta} = \theta \boldsymbol{n}$, $\|\boldsymbol{n}\| = 1$. Assuming that at some point in the calculation the knot is characterized by $(\boldsymbol{w_0}, \boldsymbol{\theta_0}, \varphi_0, \xi_0, \eta_0)$, a change $(\boldsymbol{\Delta w}, \boldsymbol{\Delta\theta}, \Delta\varphi, \Delta\xi, \Delta\eta)$ leads to (cf. Equation (45)):

$$\boldsymbol{u_0} + \boldsymbol{\Delta u} = \boldsymbol{w_0} + \boldsymbol{\Delta w} + [\boldsymbol{R}(\boldsymbol{\theta_0} + \boldsymbol{\Delta\theta}) \cdot \boldsymbol{U}(\varphi_0 + \Delta\varphi, \xi_0 + \Delta\xi, \eta_0 + \Delta\eta) - \boldsymbol{I}] \cdot (\boldsymbol{p} - \boldsymbol{q}). \tag{51}$$

Taylor expansion of $\boldsymbol{R}$:

$$\boldsymbol{R}(\boldsymbol{\theta_0} + \boldsymbol{\Delta\theta}) = \boldsymbol{R}(\boldsymbol{\theta_0}) + \left.\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\theta}}\right|_{\boldsymbol{\theta_0}} \cdot \boldsymbol{\Delta\theta} + ..., \tag{52}$$

and similar for $\boldsymbol{U}$ and keeping linear terms only leads to the following equation:

$$\begin{aligned} \boldsymbol{\Delta u} = & \boldsymbol{\Delta w} + \left[\left.\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\theta}}\right|_{\boldsymbol{\theta_0}} \cdot \boldsymbol{\Delta\theta} \right] \cdot \boldsymbol{U}(\varphi_0, \xi_0, \eta_0) \cdot (\boldsymbol{p} - \boldsymbol{q}) \\ & + \boldsymbol{R}(\boldsymbol{\theta_0}) \cdot \left[\left.\frac{\partial \boldsymbol{U}}{\partial \varphi}\right|_{\varphi_0} \Delta\varphi + \left.\frac{\partial \boldsymbol{U}}{\partial \xi}\right|_{\xi_0} \Delta\xi + \left.\frac{\partial \boldsymbol{U}}{\partial \eta}\right|_{\eta_0} \Delta\eta \right] \cdot (\boldsymbol{p} - \boldsymbol{q}) \\ & + \boldsymbol{w_0} + [\boldsymbol{R}(\boldsymbol{\theta_0}) \cdot \boldsymbol{U}(\varphi_0, \xi_0, \eta_0) - \boldsymbol{I}] \cdot (\boldsymbol{p} - \boldsymbol{q}) - \boldsymbol{u_0}. \end{aligned} \tag{53}$$

The latter equation is a inhomogeneous linear equation linking the change in displacements of an arbitrary node belonging to a knot to the change in the knot parameters (translation, rotation and stretch). This equation is taken into account at the construction phase of the governing equations. In that way the expanded degrees of freedom, being dependent, never show up in the equations to solve.

Shell knot The expansion of a shell node leads to a set of nodes lying on a straight line. Therefore, the stretch tensor $\boldsymbol{U}$ is reduced to the stretch along this line. Let $\boldsymbol{T_1}$ be a unit vector parallel to the expansion and $\boldsymbol{T_2}$ and $\boldsymbol{T_3}$ unit vectors such that $\boldsymbol{T_2} \cdot \boldsymbol{T_3} = 0$ and $\boldsymbol{T_1} \times \boldsymbol{T_2} = \boldsymbol{T_3}$. Then $\boldsymbol{U}$ can be written as:

$$\boldsymbol{U} = \alpha \boldsymbol{T_1} \otimes \boldsymbol{T_1} + \boldsymbol{T_2} \otimes \boldsymbol{T_2} + \boldsymbol{T_3} \otimes \boldsymbol{T_3} \tag{54}$$

leading to one stretch parameter α. Since the stretch along $\boldsymbol{T_2}$ and $\boldsymbol{T_3}$ is immaterial, Equation (54) can also be replaced by

$$\boldsymbol{U} = \alpha \boldsymbol{T_1} \otimes \boldsymbol{T_1} + \alpha \boldsymbol{T_2} \otimes \boldsymbol{T_2} + \alpha \boldsymbol{T_3} \otimes \boldsymbol{T_3} = \alpha \boldsymbol{I} \tag{55}$$

representing an isotropic expansion. Equation (53) can now be replaced by

$$\begin{aligned} \boldsymbol{\Delta u} = & \boldsymbol{\Delta w} + \alpha_0 \left[\left.\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\theta}}\right|_{\boldsymbol{\theta_0}} \cdot \boldsymbol{\Delta\theta} \right] \cdot (\boldsymbol{p} - \boldsymbol{q}) + \Delta\alpha \boldsymbol{R}(\boldsymbol{\theta_0}) \cdot (\boldsymbol{p} - \boldsymbol{q}) \\ & + \boldsymbol{w_0} + [\alpha_0 \boldsymbol{R}(\boldsymbol{\theta_0}) - \boldsymbol{I}] \cdot (\boldsymbol{p} - \boldsymbol{q}) - \boldsymbol{u_0}. \end{aligned} \tag{56}$$

Consequently, a knot resulting from a shell expansion is characterized by 3 translational degrees of freedom, 3 rotational degrees of freedom and 1 stretch degree of freedom.

Arbitrary knot A knot generally consists of one or more expansions of one and the same node, leading to a cloud of nodes $\boldsymbol{p_i}$. In the previous two sections knots were considered consisting of the expanded nodes of just one beam element or just one shell element. Generally, a knot will be the result of several beam and shell elements leading to a cloud of nodes in three-dimensional space. In order to determine the dimensionality of this cloud the first and second order moments of inertia are calculated leading to the location of the center of gravity and the second order moments about the center of gravity. The principal values of the second order moment matrix can be used to catalogue the dimensionality of the nodal cloud: if the lowest two principal values are zero the dimensionality is one (i.e. the nodes lie on a line as for the shell knot), if only the lowest one is zero the dimensionality is two (i.e. the nodes lie in a plane as for a beam knot). Else, the dimensionality is three. If the dimensionality corresponds to the highest dimensionality of the single elements involved, the formulation corresponding to that dimensionality is used.

If the dimensionality of the nodal cloud exceeds the highest dimensionality of the single elements, the shell knot formulation (isotropic expansion) is used. The reason for this is that the knot is supposed to be physically rigid, i.e. the relative angular position of the constituing elements should not change during deformation. Using the beam knot formulation leads to anisotropic stretching, which changes this relative angular position.

6.7.4 Node-to-Face Penalty Contact

General considerations Contact is a strongly nonlinear kind of boundary condition, preventing bodies to penetrate each other. The contact definitions implemented in CalculiX are a node-to-face penalty method and a face-to-face penalty method, both based on a pairwise interaction of surfaces. They cannot be mixed in one and the same input deck. In the present section the node-to-face penalty method is explained. For details on the penalty method the reader is referred to [75] and [40].

Each pair of interacting surfaces consists of a dependent surface and an independent surface. The dependent surface (= slave) may be defined based on nodes or element faces, the independent surface (= master) must consist of element faces (Figure 111). The element faces within one independent surface must be such, that any edge of any face has at most one neighboring face. Usually, the mesh on the dependent side should be at least as fine as on the independent side. As many pairs can be defined as needed. A contact pair is defined by the keyword card *CONTACT PAIR.

If the elements adjacent to the slave surface are quadratic elements (e.g. C3D20, C3D10 or C3D15), convergence may be slower. This especially applies to elements having quadrilateral faces in the slave surface. A uniform pressure

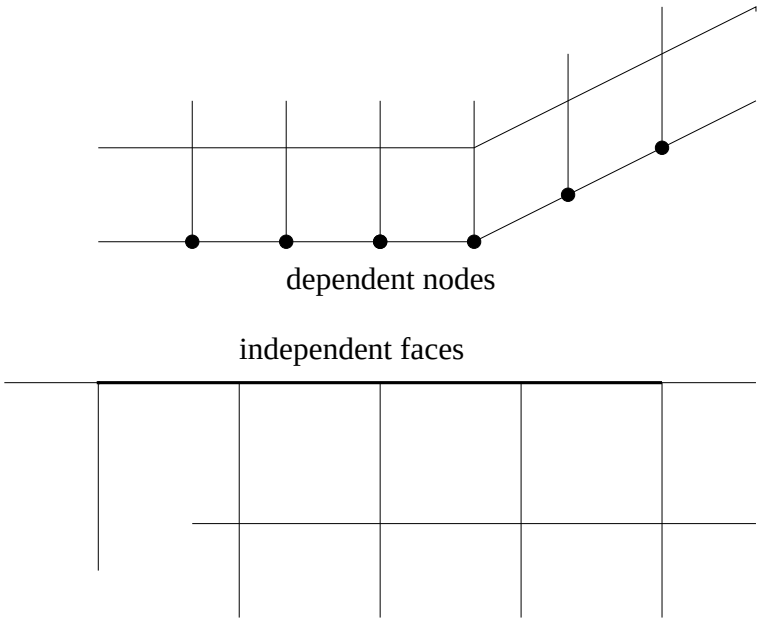


Figure 111: Definition of the dependent nodal surface and the independent element face surface

on a quadratic (8-node) quadrilateral face leads to compressive forces in the midnodes and tensile forces in the vertex nodes [18] (with weights of 1/3 and -1/12, respectively). The tensile forces in the corner nodes usually lead to divergence if this node belongs to a node-to-face contact element. Therefore, in CalculiX the weights are modified into 24/100 and 1/100, respectively. In general, node-to-face contact is not recommended for quadratic elements. Instead, face-to-face contact should be used.

In CalculiX, penalty contact is modeled by the generation of (non)linear spring elements. To this end, for each node on the dependent surface, a face on the independent surface is localized such that it contains the orthogonal projection of the node. If such is face is found a nonlinear spring element is generated consisting of the dependent node and all vertex nodes belonging to the independent face (Figure 112). Depending of the kind of face the contact spring element contains 4, 5, 7 or 9 nodes. The properties of the spring are defined by a *SURFACE INTERACTION definition, whose name must be specified on the *CONTACT PAIR card.

The user can determine how often during the calculation the pairing of the dependent nodes with the independent faces takes place. If the user specifies the parameter SMALL SLIDING on the *CONTACT PAIR card, the pairing is done once per increment. If this parameter is not selected, the pairing is checked every iteration for all iterations below 9, for iterations 9 and higher the contact elements are frozen to improve convergence. Deactivating SMALL SLIDING is

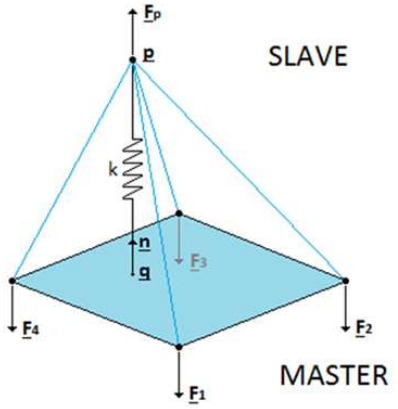


Figure 112: Creation of a node-to-face penalty contact element

useful if the sliding is particularly large.

The *SURFACE INTERACTION keyword card is very similar to the *MATERIAL card: it starts the definition of interaction properties in the same way a *MATERIAL card starts the definition of material properties. Whereas material properties are characterized by cards such as *DENSITY or *ELASTIC, interaction properties are denoted by the *SURFACE BEHAVIOR and the *FRICTION card. All cards beneath a *SURFACE INTERACTION card are interpreted as belonging to the surface interaction definition until a keyword card is encountered which is not a surface interaction description card. At that point, the surface interaction description is considered to be finished. Consequently, an interaction description is a closed block in the same way as a material description, Figure 3.

The *SURFACE BEHAVIOR card defines the linear (actually quasi bilinear as illustrated by Figure 114), exponential, or piecewice linear normal (i.e. locally perpendicular onto the master surface) behavior of the spring element. The pressure p exerted on the independent face of a contact spring element with exponential behavior is given by

$$p = p_0 \exp(\beta d), \tag{57}$$

where p_0 is the pressure at zero clearance, β is a coefficient and d is the overclosure (penetration of the slave node into the master side; a negative penetration is a clearance). Instead of having to specify β, which lacks an immediate physical significance, the user is expected to specify c_0 which is the clearance at which the pressure is 1 % of p_0. From this β can be calculated:

$$\beta = \frac{\ln 100}{c_0}. \tag{58}$$

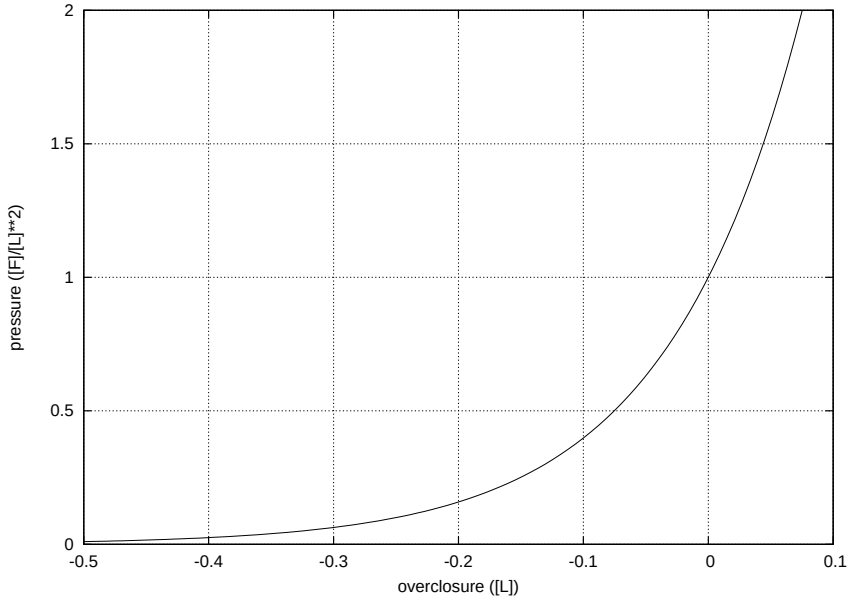


Figure 113: Exponential pressure-overclosure relationship

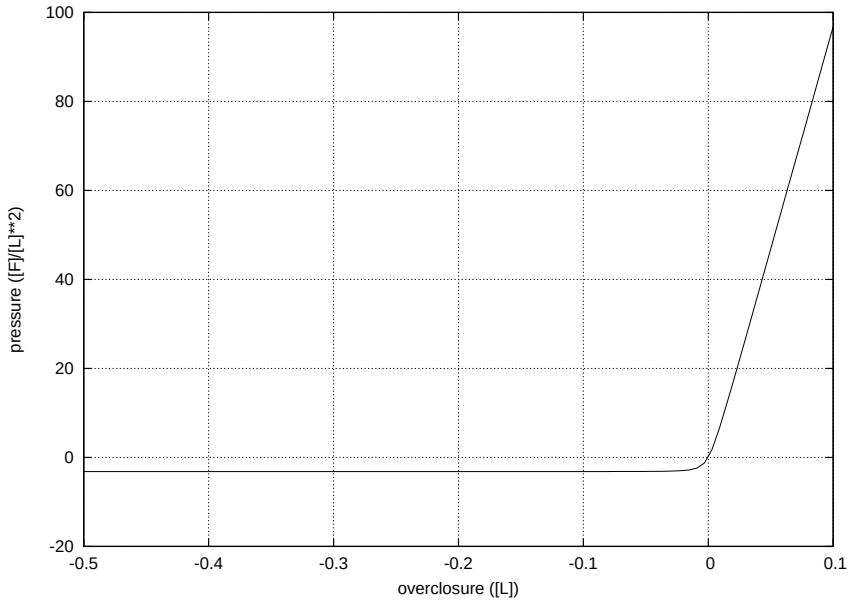


Figure 114: Linear pressure-overclosure relationship

The pressure curve for $p_0 = 1$ and $c_0 = 0.5$ looks like in Figure 113. A large value of c_0 leads to soft contact, i.e. large penetrations can occur, hard contact is modeled by a small value of c_0. Hard contact leads to slower convergence than soft contact. If the distance of the slave node to the master surface exceeds c_0 no contact spring element is generated. For exponential behavior the user has to specify c_0 and p_0 underneath the *SURFACE BEHAVIOR card.

In case of a linear contact spring the pressure-overclosure relationship is given by

$$p = Kd \left[\frac{1}{2} + \frac{1}{\pi} \tan^{-1} \left(\frac{d}{\epsilon} \right) \right], \tag{59}$$

were ϵ is a small number. The term in square brackets makes sure that the value of p is very small for $d \leq 0$. In general, a linear contact spring formulation will converge more easily than an exponential behavior. The pressure curve for $K = 10^3$ and $\epsilon = 10^{-2}$ looks like in Figure 114. A large value of K leads to hard contact. To obtain good results K should typically be 5 to 50 times the E-modulus of the adjacent materials. If one knows the roughness of the contact surfaces in the form of a peak-to-valley distance d_{pv} and the maximum pressure p_{max} to expect, one might estimate the spring constant by $K = p_{max}/d_{pv}$. The units of K are [Force]/[Length]^3.

Notice that for a large negative overclosure a tension σ_∞ results (for $d \to -\infty$), equal to $K\epsilon/\pi$. The value of σ_∞ has to be specified by the user. A good value is about 0.25 % of the maximum expected stress in the model. CalculiX calculates ϵ from σ_∞ and K.

For a linear contact spring the distance beyond which no contact spring element is generated is defined by $c_0\sqrt{\text{spring area}}$ if the spring area exceeds zero, and 10^{-10} otherwise. The default for c_0 is 10^{-3} (dimensionless) but may be changed by the user. For a linear pressure-overclosure relationship the user has to specify K and σ_∞ underneath the *SURFACE BEHAVIOR card. c_0 is optional, and may be entered as the third value on the same line.

The pressure-overclosure behavior can also be defined as a piecewise linear function (PRESSURE-OVERCLOSURE=TABULAR). In this way the user can use experimental data to define the curve. For a tabular spring the distance beyond which no contact spring element is generated is defined by $10^{-3}\sqrt{\text{spring area}}$ if the spring area exceeds zero, and 10^{-10} otherwise. For tabular behavior the user has to enter pressure-overclosure pairs, one on a line.

The normal spring force is defined as the pressure multiplied by the spring area. The spring area is assigned to the slave nodes and defined by 1/4 (linear quadrilateral faces) or 1/3 (linear triangular faces) of the slave faces the slave node belongs to. For quadratic quadrilateral faces the weights are 24/100 for middle nodes and 1/100 for corner nodes. For quadratic triangular faces these weight are 1/3 and 0, respectively.

The tangential spring force is defined as the shear stress multiplied by the spring area. The shear stress is a function of the relative displacement $\|\boldsymbol{t}\|$ between the slave node and the master face. This function is shown in Figure

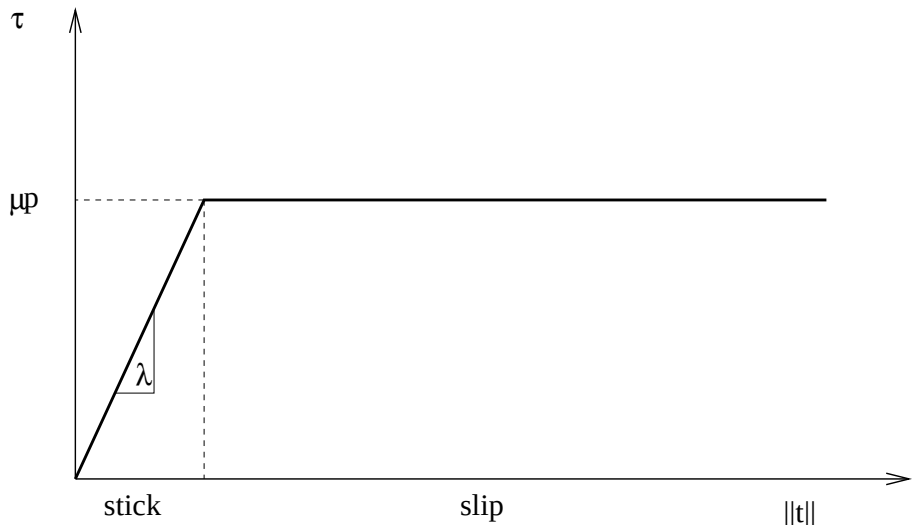


Figure 115: Shear stress versus relative tangential displacement

115. It consists of a stick range, in which the shear stress is a linear function of the relative tangential displacement, and a slip range, for which the shear stress is a function of the local pressure only. User input consists of the friction coefficient μ which is dimensionless and usually takes values between 0.1 and 0.5 and the stick slope λ which has the dimension of force per unit of volume and should be chosen about 100 times smaller than the spring constant.

The friction can be redefined in all but the first step by the *CHANGE FRICTION keyword card. In the same way contact pairs can be activated or deactivated in all but the first step by using the *MODEL CHANGE card.

If CalculiX detects an overlap of the contacting surfaces at the start of a step, the overlap is completely taken into account at the start of the step for a dynamic calculation (*DYNAMIC or *MODAL DYNAMIC) whereas it is linearly ramped for a static calculation (*STATIC).

Finally a few useful rules if you experience convergence problems:

- Deactivate NLGEOM (i.e. do not use NLGEOM on the *STEP card). Recall, however, that NLGEOM is activated automatically if you have nonlinear material behavior.
- Try SMALL SLIDING first, and then large sliding, if applicable.
- Try a linear pressure-overclosure relationship first (instead of exponential), with a stiffness constant about 5 to 50 times Young's modulus of the adjacent materials.
- Define your slave surface based on faces, not on nodes. This can be especially helpful if you use quadratic elements.

- Make sure that the mesh density on the slave side is at least as fine as on the master side, preferably finer.
- Deactivate friction first.

Notice that the parameter CONTACT ELEMENTS on the *NODE FILE, *EL FILE, NODE OUTPUT, or *ELEMENT OUTPUT card stores the contact elements which have been generated in each iteration as a set with the name contactelements_stα_inβ_atγ_itδ (where α is the step number, β the increment number, γ the attempt number and δ the iteration number) in a file "contactelements.inp". When opening the frd file with CalculiX GraphiX this file can be read with the command "read contactelements.inp" and visualized by plotting the elements in the appropriate set. These elements are the contact spring elements and connect the slave nodes with the corresponding master surfaces. In case of contact these elements will be very flat. Moving the parts apart (by a translation) will improve the visualization. Using the screen up and screen down key one can check how contact evolved during the calculation. Looking at where contact elements have been generated may help localizing the problem in case of divergence.

Notice that the number of contact elements generated is also listed in the screen output for each iteration in which contact was established anew, i.e. for each iteration ≤ 8 if the SMALL SLIDING parameter was not used on the *CONTACT PAIR card, else only in the first iteration of each increment.

Normal contact stiffness A node-to-face contact element consists of a slave node connected to a master face (cf. Figure 112). Therefore, it consists of $1 + n_m$ nodes, where n_m is the number of nodes belonging to the master face. The stiffness matrix of a finite element is the derivative of the internal forces in each of the nodes w.r.t. the displacements of each of the nodes. Therefore, we need to determine the internal force in the nodes.

Denoting the position of the slave node by $\boldsymbol{p}$ and the position of the projection onto the master face by $\boldsymbol{q}$, the vector connecting both satisfies:

$$\boldsymbol{r} = \boldsymbol{p} - \boldsymbol{q}. \tag{60}$$

The clearance r at this position can be described by

$$r = \boldsymbol{r} \cdot \boldsymbol{n} \tag{61}$$

where $\boldsymbol{n}$ is the local normal on the master face. Denoting the nodes belonging to the master face by $\boldsymbol{q_i}, i = 1, n_m$ and the local coordinates within the face by ξ and η, one can write:

$$\boldsymbol{q} = \sum_j \varphi_j(\xi, \eta)\boldsymbol{q_j}, \tag{62}$$

$$\boldsymbol{m} = \frac{\partial \boldsymbol{q}}{\partial \xi} \times \frac{\partial \boldsymbol{q}}{\partial \eta} \tag{63}$$

and

$$\boldsymbol{n} = \frac{\boldsymbol{m}}{\|\boldsymbol{m}\|}. \tag{64}$$

$\boldsymbol{m}$ is the Jacobian vector on the surface. The internal force on node p is now given by

$$\boldsymbol{F_p} = -f(r)\boldsymbol{n}a_p, \tag{65}$$

where f is the pressure versus clearance function selected by the user and a_p is the slave area for which node p is representative. If the slave node belongs to N contact slave faces i with area A_i, this area may be calculated as:

$$a_p = \sum_{i=1}^{N} A_i/n_{si}. \tag{66}$$

The minus sign in Equation (65) stems from the fact that the internal force is minus the external force (the external force is the force the master face exerts on the slave node). Replacing the normal in Equation (65) by the Jacobian vector devided by its norm and taking the derivative w.r.t. $\boldsymbol{u_i}$, where i can be the slave node or any node belonging to the master face one obtains:

$$\frac{1}{a_p}\frac{\partial \boldsymbol{F_p}}{\partial \boldsymbol{u_i}} = -\frac{\boldsymbol{m}}{\|\boldsymbol{m}\|}\otimes\frac{\partial f}{\partial r}\left[\frac{\partial}{\partial \boldsymbol{u_i}}\left(\frac{\boldsymbol{m}}{\|\boldsymbol{m}\|}\cdot\boldsymbol{r}\right)\right] - \frac{f}{\|\boldsymbol{m}\|}\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{u_i}} + \frac{f}{\|\boldsymbol{m}\|^2}\boldsymbol{m}\otimes\frac{\partial\|\boldsymbol{m}\|}{\partial \boldsymbol{u_i}}. \tag{67}$$

Since

$$\frac{\partial}{\partial \boldsymbol{u_i}}\left(\frac{\boldsymbol{m}}{\|\boldsymbol{m}\|}\cdot\boldsymbol{r}\right) = \frac{1}{\|\boldsymbol{m}\|}\,\boldsymbol{r}\cdot\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{u_i}} - \frac{r}{\|\boldsymbol{m}\|}\frac{\partial\|\boldsymbol{m}\|}{\partial \boldsymbol{u_i}} + \frac{\boldsymbol{m}}{\|\boldsymbol{m}\|}\cdot\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u_i}}, \tag{68}$$

the above equation can be rewritten as

$$\begin{aligned}\frac{1}{a_p}\frac{\partial \boldsymbol{F_p}}{\partial \boldsymbol{u_i}} = &-\left(\frac{\partial f}{\partial r}\frac{1}{\|\boldsymbol{m}\|^2}\right)\boldsymbol{m}\otimes\left[\boldsymbol{r}\cdot\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{u_i}} + \boldsymbol{m}\cdot\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u_i}} - r\frac{\partial\|\boldsymbol{m}\|}{\partial \boldsymbol{u_i}}\right] \\ &+ \frac{f}{\|\boldsymbol{m}\|}\left[\boldsymbol{n}\otimes\frac{\partial\|\boldsymbol{m}\|}{\partial \boldsymbol{u_i}} - \frac{\partial \boldsymbol{m}}{\partial \boldsymbol{u_i}}\right].\end{aligned} \tag{69}$$

Consequently, the derivatives which are left to be determined are $\partial\boldsymbol{m}/\partial\boldsymbol{u_i}$, $\partial\boldsymbol{r}/\partial\boldsymbol{u_i}$ and $\partial\|\boldsymbol{m}\|/\partial\boldsymbol{u_i}$.

The derivative of $\boldsymbol{m}$ is obtained by considering Equation (63), which can also be written as:

$$\boldsymbol{m} = \sum_j\sum_k \frac{\partial\varphi_j}{\partial\xi}\frac{\partial\varphi_k}{\partial\eta}[\boldsymbol{q_j}\times\boldsymbol{q_k}]. \tag{70}$$

Derivation yields (notice that ξ and η are a function of $\boldsymbol{u_i}$, and that $\partial\boldsymbol{q_i}/\partial\boldsymbol{u_j} = \delta_{ij}\boldsymbol{I}$) :

$$\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{u_i}} = \left[\frac{\partial^2 \boldsymbol{q}}{\partial \xi^2} \times \frac{\partial \boldsymbol{q}}{\partial \eta} + \frac{\partial \boldsymbol{q}}{\partial \xi} \times \frac{\partial^2 \boldsymbol{q}}{\partial \xi \partial \eta}\right] \otimes \frac{\partial \xi}{\partial \boldsymbol{u_i}} + \left[\frac{\partial \boldsymbol{q}}{\partial \xi} \times \frac{\partial^2 \boldsymbol{q}}{\partial \eta} + \frac{\partial^2 \boldsymbol{q}}{\partial \xi \partial \eta} \times \frac{\partial \boldsymbol{q}}{\partial \eta}\right] \otimes \frac{\partial \eta}{\partial \boldsymbol{u_i}} + \sum_{j=1}^{n_m}\sum_{k=1}^{n_m}\left[\frac{\partial \varphi_j}{\partial \xi}\frac{\partial \varphi_k}{\partial \eta} - \frac{\partial \varphi_k}{\partial \xi}\frac{\partial \varphi_j}{\partial \eta}\right](\boldsymbol{I} \times \boldsymbol{q_k})\delta_{ij}, \quad i = 1, ..n_m; p \tag{71}$$

The derivatives $\partial\xi/\partial \boldsymbol{u_i}$ and $\partial\eta/\partial \boldsymbol{u_i}$ on the right hand side are unknown and will be determined later on. They represent the change of ξ and η whenever any of the $\boldsymbol{u_i}$ is changed, k being the slave node or any of the nodes belonging to the master face. Recall that the value of ξ and η is obtained by orthogonal projection of the slave node on the master face.

Combining Equations (60) and (62) to obtain $\boldsymbol{r}$, the derivative w.r.t. $\boldsymbol{u_i}$ can be written as:

$$\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u_i}} = \delta_{ip}\boldsymbol{I} - \left[\frac{\partial \boldsymbol{q}}{\partial \xi} \otimes \frac{\partial \xi}{\partial \boldsymbol{u_i}} + \frac{\partial \boldsymbol{q}}{\partial \eta} \otimes \frac{\partial \eta}{\partial \boldsymbol{u_i}} + \varphi_i(1 - \delta_{ip})\boldsymbol{I}\right], \tag{72}$$

where p represents the slave node.

Finally, the derivative of the norm of a vector can be written as a function of the derivative of the vector itself:

$$\frac{\partial \|\boldsymbol{m}\|}{\partial \boldsymbol{u_i}} = \frac{\boldsymbol{m}}{\|\boldsymbol{m}\|} \cdot \frac{\partial \boldsymbol{m}}{\partial \boldsymbol{u_i}}. \tag{73}$$

The only derivatives left to determine are the derivatives of ξ and η w.r.t. $\boldsymbol{u_i}$. Requiring that $\boldsymbol{q}$ is the orthogonal projection of $\boldsymbol{p}$ onto the master face is equivalent to expressing that the connecting vector $\boldsymbol{r}$ is orthogonal to the vectors $\partial\boldsymbol{q}/\partial\xi$ and $\partial\boldsymbol{q}/\partial\eta$, which are tangent to the master surface.
Now,

$$\boldsymbol{r} \perp \frac{\partial \boldsymbol{q}}{\partial \xi} \tag{74}$$

can be rewritten as

$$\boldsymbol{r} \cdot \frac{\partial \boldsymbol{q}}{\partial \xi} = 0 \tag{75}$$

or

$$\left[\boldsymbol{p} - \sum_i \varphi_i(\xi, \eta)\boldsymbol{q_i}\right] \cdot \left[\sum_i \frac{\partial \varphi_i}{\partial \xi}\boldsymbol{q_i}\right] = 0. \tag{76}$$

Differentation of the above expression leads to

$$\left[d\boldsymbol{p} - \sum_i \left(\frac{\partial \varphi_i}{\partial \xi}\boldsymbol{q_i}d\xi + \frac{\partial \varphi_i}{\partial \eta}\boldsymbol{q_i}d\eta + \varphi_i d\boldsymbol{q_i}\right)\right] \cdot \boldsymbol{q_\xi} +$$
$$\boldsymbol{r} \cdot \left[\sum_i \left(\frac{\partial^2 \varphi_i}{\partial \xi^2}\boldsymbol{q_i}d\xi + \frac{\partial^2 \varphi_i}{\partial \xi \partial \eta}\boldsymbol{q_i}d\eta + \frac{\partial \varphi_i}{\partial \xi}d\boldsymbol{q_i}\right)\right] = 0 \tag{77}$$

where $\boldsymbol{q_\xi}$ is the derivative of $\boldsymbol{q}$ w.r.t. ξ. The above equation is equivalent to:

$$(d\boldsymbol{p} - \boldsymbol{q}_\xi d\xi - \boldsymbol{q}_\eta d\eta - \sum_i \varphi_i d\boldsymbol{q_i}) \cdot \boldsymbol{q}_\xi +$$
$$\boldsymbol{r} \cdot (\boldsymbol{q}_{\xi\xi}d\xi + \boldsymbol{q}_{\xi\eta}d\eta + \sum_i \frac{\partial \varphi_i}{\partial \xi}d\boldsymbol{q_i}) = 0. \tag{78}$$

One finally arrives at:

$$(-\boldsymbol{q}_\xi \cdot \boldsymbol{q}_\xi + \boldsymbol{r} \cdot \boldsymbol{q}_{\xi\xi})d\xi + (-\boldsymbol{q}_\eta \cdot \boldsymbol{q}_\xi + \boldsymbol{r} \cdot \boldsymbol{q}_{\xi\eta})d\eta =$$
$$-\boldsymbol{q}_\xi \cdot d\boldsymbol{p} + \sum_i \left[(\varphi_i \boldsymbol{q}_\xi - \frac{\partial \varphi_i}{\partial \xi}\boldsymbol{r}) \cdot d\boldsymbol{q_i}\right] \tag{79}$$

and similarly for the tangent in η-direction:

$$(-\boldsymbol{q}_\xi \cdot \boldsymbol{q}_\eta + \boldsymbol{r} \cdot \boldsymbol{q}_{\xi\eta})d\xi + (-\boldsymbol{q}_\eta \cdot \boldsymbol{q}_\eta + \boldsymbol{r} \cdot \boldsymbol{q}_{\eta\eta})d\eta =$$
$$-\boldsymbol{q}_\eta \cdot d\boldsymbol{p} + \sum_i \left[(\varphi_i \boldsymbol{q}_\eta - \frac{\partial \varphi_i}{\partial \eta}\boldsymbol{r}) \cdot d\boldsymbol{q_i}\right] \tag{80}$$

From this $\partial\xi/\partial\boldsymbol{q_i}$, $\partial\xi/\partial\boldsymbol{p}$ and so on can be determined. Indeed, suppose that all $d\boldsymbol{q_i}, i = 1, .., n_m = \boldsymbol{0}$ and $dp_y = dp_z = 0$. Then, the right hand side of the above equations reduces to $-\boldsymbol{q_{\xi}}_x dp_x$ and $-\boldsymbol{q_{\eta}}_x dp_x$ and one ends up with two equations in the two unknowns $\partial\xi/\partial p_x$ and $\partial\eta/\partial p_x$. Once $\partial\xi/\partial\boldsymbol{p}$ is determined one automatically obtains $\partial\xi/\partial\boldsymbol{u_p}$ since

$$\frac{\partial \xi}{\partial \boldsymbol{p}} = \frac{\partial \xi}{\partial \boldsymbol{u_p}}, \tag{81}$$

and similarly for the other derivatives. This concludes the derivation of $\partial\boldsymbol{F}_p/\partial\boldsymbol{u_i}$. Since

$$\boldsymbol{F_j} = -\varphi_j(\xi, \eta)\boldsymbol{F_p}, \tag{82}$$

one obtains:

$$\frac{\partial \boldsymbol{F_j}}{\partial \boldsymbol{u_i}} = -\boldsymbol{F_p} \otimes \left[\frac{\partial \varphi_j}{\partial \xi}\frac{\partial \xi}{\partial \boldsymbol{u_i}} + \frac{\partial \varphi_j}{\partial \eta}\frac{\partial \eta}{\partial \boldsymbol{u_i}}\right] - \varphi_j \frac{\partial \boldsymbol{F_p}}{\partial \boldsymbol{u_i}} \tag{83}$$

for the derivatives of the forces in the master nodes.

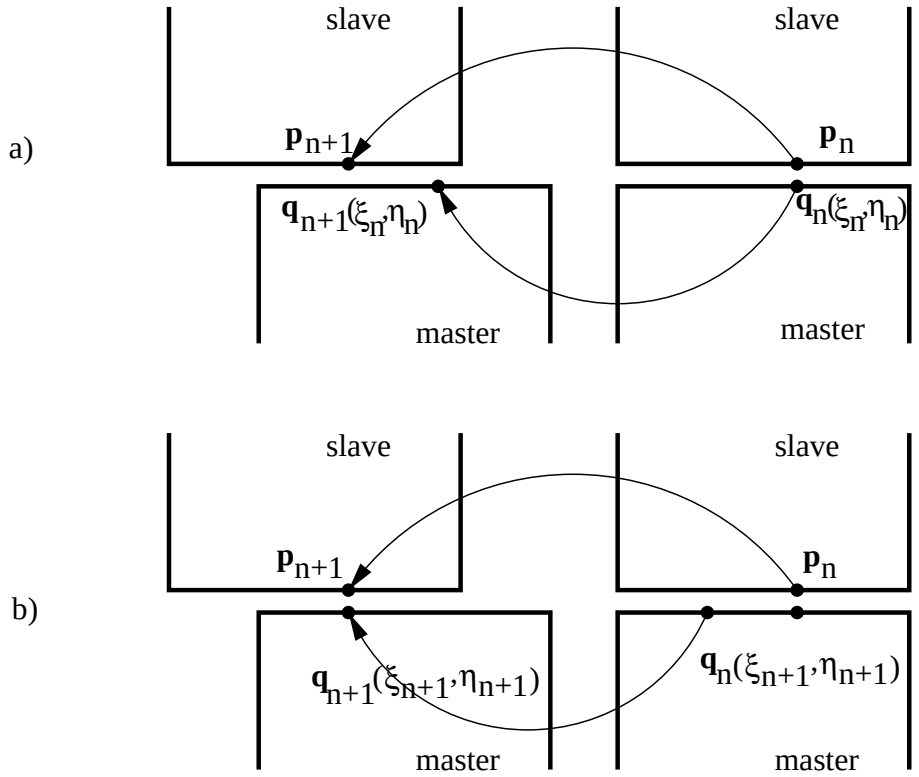


Figure 116: Visualization of the tangential differential displacements

Tangent contact stiffness To find the tangent contact stiffness matrix, please look at Figure 116, part a). At the beginning of a concrete time increment, characterized by time t_n, the slave node at position $\boldsymbol{p}_n$ corresponds to the projection vector $\boldsymbol{q}_n$ on the master side. At the end of the time increment, characterized by time t_{n+1} both have moved to positions $\boldsymbol{p}_{n+1}$ and $\boldsymbol{q}_{n+1}$, respectively. The differential displacements changed during this increment by the vector $\boldsymbol{s}$ satisfying:

$$\boldsymbol{s} = (\boldsymbol{p}_{n+1} - \boldsymbol{q}_{n+1}) - (\boldsymbol{p}_n - \boldsymbol{q}_n). \tag{84}$$

Here, $\boldsymbol{q_{n+1}}$ satisfies

$$\boldsymbol{q}_{n+1} = \sum_j \varphi_j(\xi_n^m, \eta_n^m)\boldsymbol{q_j}_{n+1}. \tag{85}$$

Notice that the local coordinates take the values of time t_n. The differential tangential displacement is changed by:

$$\boldsymbol{t} = \boldsymbol{s} - s\boldsymbol{n}, \tag{86}$$

where

$$s = \boldsymbol{s} \cdot \boldsymbol{n}. \tag{87}$$

Derivation w.r.t. $\boldsymbol{u_i}$ satisfies (straightforward differentiation):

$$\frac{\partial \boldsymbol{t}}{\partial \boldsymbol{u_i}} = \frac{\partial \boldsymbol{s}}{\partial \boldsymbol{u_i}} - \boldsymbol{n} \otimes \frac{\partial s}{\partial \boldsymbol{u_i}} - s\frac{\partial \boldsymbol{n}}{\partial \boldsymbol{u_i}} \tag{88}$$

$$\frac{\partial s}{\partial \boldsymbol{u_i}} = \frac{\boldsymbol{s}}{\|\boldsymbol{m}\|} \cdot \frac{\partial \boldsymbol{m}}{\partial \boldsymbol{u_i}} - \frac{s}{\|\boldsymbol{m}\|}\frac{\partial \|\boldsymbol{m}\|}{\boldsymbol{u_i}} + \frac{\boldsymbol{m}}{\|\boldsymbol{m}\|} \cdot \frac{\partial \boldsymbol{s}}{\partial \boldsymbol{u_i}} \tag{89}$$

and

$$\frac{\partial \boldsymbol{n}}{\partial \boldsymbol{u_i}} = \frac{1}{\|\boldsymbol{m}\|}\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{u_i}} - \frac{1}{\|\boldsymbol{m}\|^2}\boldsymbol{m} \otimes \frac{\partial \|\boldsymbol{m}\|}{\boldsymbol{u_i}}. \tag{90}$$

The derivative of $\boldsymbol{s}$ w.r.t. $\boldsymbol{u_i}$ can be obtained from the derivative of $\boldsymbol{r}$ w.r.t. $\boldsymbol{u_i}$ by keeping ξ and η fixed (notice that the derivative is taken at t_{n+1}, consequently, all derivatives of values at time t_n disappear):

$$\frac{\partial \boldsymbol{s}}{\partial \boldsymbol{u_i}} = \delta_{ip}\boldsymbol{I} - \varphi_i(1 - \delta_{ip})\boldsymbol{I}. \tag{91}$$

Physically, the tangential contact equations are as follows (written at the location of slave node p):

- an additive decomposition of the differential tangential displacement in stick $\boldsymbol{t^3}$ and slip $\boldsymbol{t^p}$:

$$\boldsymbol{t} = \boldsymbol{t^e} + \boldsymbol{t^p}. \tag{92}$$

- a stick law ($K_t \equiv \lambda a_p$, where λ is the stick slope and a_p the representative slave area for the slave node at stake) defining the tangential force exerted by the slave side on the master side at the location of slave node p:

$$\boldsymbol{F_T} = K_t \boldsymbol{t^e}. \tag{93}$$

- a Coulomb slip limit:

$$\|\boldsymbol{F_T}\| \leq \mu \|\boldsymbol{F_N}\| \tag{94}$$

- a slip evolution equation:

$$\dot{\boldsymbol{t}}^{\boldsymbol{p}} = \dot{\gamma} \frac{\boldsymbol{F_T}}{\|\boldsymbol{F_T}\|} \tag{95}$$

First, a difference form of the additive decomposition of the differential tangential displacement is derived. Starting from

$$\boldsymbol{t} = \boldsymbol{t^e} + \boldsymbol{t^p}, \tag{96}$$

one obtains after taking the time derivative:

$$\dot{\boldsymbol{t}} = \dot{\boldsymbol{t}}^{\boldsymbol{e}} + \dot{\boldsymbol{t}}^{\boldsymbol{p}}. \tag{97}$$

Substituting the slip evolution equation leads to:

$$\dot{\gamma} \frac{\boldsymbol{F_T}}{\|\boldsymbol{F_T}\|} = \dot{\boldsymbol{t}} - \dot{\boldsymbol{t}}^{\boldsymbol{e}}, \tag{98}$$

and after multiplying with K_t:

$$K_t \dot{\gamma} \frac{\boldsymbol{F_T}}{\|\boldsymbol{F_T}\|} = K_t \dot{\boldsymbol{t}} - K_t \dot{\boldsymbol{t}}^{\boldsymbol{e}} \tag{99}$$

Writing this equation at t_{n+1}, using finite differences (backwards Euler), one gets:

$$K_t \Delta\gamma_{n+1} \frac{\boldsymbol{F_T}_{n+1}}{\|\boldsymbol{F_T}_{n+1}\|} = K_t \Delta \boldsymbol{t}_{n+1} - K_t \boldsymbol{t^e}_{n+1} + K_t \boldsymbol{t^e}_n, \tag{100}$$

where $\Delta\gamma_{n+1} \equiv \dot{\gamma}_{n+1} \Delta t$ and $\Delta \boldsymbol{t}_{n+1} \equiv \boldsymbol{t}_{n+1} - \boldsymbol{t}_n$. The parameter K_t is assumed to be independent of time.

Now, the radial return algorithm will be described to solve the governing equations. Assume that the solution at time t_n is known, i.e. $\boldsymbol{t^e}_n$ and $\boldsymbol{t^p}_n$ are known. Using the stick law the tangential forc $\boldsymbol{F_T}_n$ can be calculated. Now we would like to know these variables at time t_{n+1}, given the total differential tangential displacement $\boldsymbol{t_{n+1}}$. At first we construct a trial tangential force $\boldsymbol{F_T}^{trial}_{n+1}$ which is the force which arises at time t_{n+1} assuming that no slip takes

place from t_n till t_{n+1}. This assumption is equivalent to $\boldsymbol{t^p}_{n+1} = \boldsymbol{t^p}_n$. Therefore, the trial tangential force satisfies (cf. the stick law):

$$\boldsymbol{F_T}^{trial}_{n+1} = K_t(\boldsymbol{t}_{n+1} - \boldsymbol{t^p}_n). \tag{101}$$

Now, this can also be written as:

$$\boldsymbol{F_T}^{trial}_{n+1} = K_t(\boldsymbol{t}_{n+1} - \boldsymbol{t}_n + \boldsymbol{t}_n - \boldsymbol{t^p}_n). \tag{102}$$

or

$$\boldsymbol{F_T}^{trial}_{n+1} = K_t\Delta\boldsymbol{t}_{n+1} + K_t\boldsymbol{t^e}_n. \tag{103}$$

Using Equation (100) this is equivalent to:

$$\boldsymbol{F_T}^{trial}_{n+1} = K_t\Delta\gamma_{n+1}\frac{\boldsymbol{F_T}_{n+1}}{\|\boldsymbol{F_T}_{n+1}\|} + K_t\boldsymbol{t^e}_{n+1}, \tag{104}$$

or

$$\boldsymbol{F_T}^{trial}_{n+1} = (K_t\Delta\gamma_{n+1}\frac{1}{\|\boldsymbol{F_T}_{n+1}\|} + 1)\boldsymbol{F_T}_{n+1}. \tag{105}$$

From the last equation one obtains

$$\boldsymbol{F_T}^{trial}_{n+1} \parallel \boldsymbol{F_T}_{n+1} \tag{106}$$

and, since the terms in brackets in Equation (105) are both positive:

$$\|\boldsymbol{F_T}^{trial}_{n+1}\| = K_t\Delta\gamma_{n+1} + \|\boldsymbol{F_T}_{n+1}\|. \tag{107}$$

The only equation which is left to be satisfied is the Coulomb slip limit. Two possibilities arise:

1. $\|\boldsymbol{F_T}^{trial}_{n+1}\| \leq \mu\|\boldsymbol{F_N}_{n+1}\|$.

   In that case the Coulomb slip limit is satisfied and we have found the solution:

   $$\boldsymbol{F_T}_{n+1} = \boldsymbol{F_T}^{trial}_{n+1} = K_t(\boldsymbol{t_{n+1}} - \boldsymbol{t^p}_n) \tag{108}$$

   and

   $$\frac{\partial\boldsymbol{F_T}_{n+1}}{\partial\boldsymbol{t}_{n+1}} = K_t\boldsymbol{I}. \tag{109}$$

   No extra slip occurred from t_n to t_{n+1}.

2. $\|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}\| > \mu\|\boldsymbol{F}_{\boldsymbol{N}}{}_{n+1}\|$.

   In that case we project the solution back onto the slip surface and require $\|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}\| = \mu\|\boldsymbol{F}_{\boldsymbol{N}}{}_{n+1}\|$. Using Equation (107) this leads to the following expression for the increase of the consistency parameter γ:

$$\Delta\gamma_{n+1} = \frac{\|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}\| - \mu\|\boldsymbol{F}_{\boldsymbol{N}}{}_{n+1}\|}{K_t}, \tag{110}$$

   which can be used to update $\boldsymbol{t}^{\boldsymbol{p}}$ (by using the slip evolution equation):

$$\Delta\boldsymbol{t}^{\boldsymbol{p}} = \Delta\gamma_{n+1}\frac{\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}}{\|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}\|} = \Delta\gamma_{n+1}\frac{\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}}{\|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}\|} \tag{111}$$

   The tangential force can be written as:

$$\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1} = \|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}\|\frac{\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}}{\|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}\|} = \mu\|\boldsymbol{F}_{\boldsymbol{N}}{}_{n+1}\|\frac{\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}}{\|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}\|}. \tag{112}$$

   Now since

$$\frac{\partial\|\boldsymbol{a}\|}{\partial\boldsymbol{b}} = \frac{\boldsymbol{a}}{\|\boldsymbol{a}\|}\cdot\frac{\partial\boldsymbol{a}}{\partial\boldsymbol{b}} \tag{113}$$

   and

$$\frac{\partial}{\partial\boldsymbol{b}}\left(\frac{\boldsymbol{a}}{\|\boldsymbol{a}\|}\right) = \frac{1}{\|\boldsymbol{a}\|}\left[\boldsymbol{I} - \left(\frac{\boldsymbol{a}}{\|\boldsymbol{a}\|}\right)\otimes\left(\frac{\boldsymbol{a}}{\|\boldsymbol{a}\|}\right)\right]\cdot\frac{\partial\boldsymbol{a}}{\partial\boldsymbol{b}}, \tag{114}$$

   where $\boldsymbol{a}$ and $\boldsymbol{b}$ are vectors, one obtains for the derivative of the tangential force:

$$\begin{aligned}\frac{\partial\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}}{\partial\boldsymbol{t}_{n+1}} &= \mu\boldsymbol{\xi}_{n+1}\otimes\left[\frac{\boldsymbol{F}_{\boldsymbol{N}}{}_{n+1}}{\|\boldsymbol{F}_{\boldsymbol{N}}{}_{n+1}\|}\cdot\frac{\partial\boldsymbol{F}_{\boldsymbol{N}}{}_{n+1}}{\partial\boldsymbol{t}_{n+1}}\right] \\ &\quad + \mu\frac{\|\boldsymbol{F}_{\boldsymbol{N}}{}_{n+1}\|}{\|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}\|}[\boldsymbol{I} - \boldsymbol{\xi}_{n+1}\otimes\boldsymbol{\xi}_{n+1}]\cdot\frac{\partial\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}}{\partial\boldsymbol{t}_{n+1},}\end{aligned} \tag{115}$$

   where

$$\boldsymbol{\xi}_{n+1} \equiv \frac{\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}}{\|\boldsymbol{F}_{\boldsymbol{T}}{}_{n+1}^{trial}\|}. \tag{116}$$

   One finally arrives at (using Equation (109)

$$\frac{\partial \boldsymbol{F_T}_{n+1}}{\partial \boldsymbol{u_i}_{n+1}} = \mu \boldsymbol{\xi}_{n+1} \otimes \left[-\boldsymbol{n} \cdot \frac{\partial \boldsymbol{F_N}_{n+1}}{\partial \boldsymbol{u_i}_{n+1}} \right] + \mu \frac{\|\boldsymbol{F_N}_{n+1}\|}{\|\boldsymbol{F_T}^{trial}_{n+1}\|} [\boldsymbol{I} - \boldsymbol{\xi}_{n+1} \otimes \boldsymbol{\xi}_{n+1}] \cdot K_t \frac{\partial \boldsymbol{t}_{n+1}}{\partial \boldsymbol{u_i}_{n+1}}. \tag{117}$$

All quantities on the right hand side are known now (cf. Equation (69) and Equation (88)).

In CalculiX, for node-to-face contact, Equation (84) is reformulated and simplified. It is reformulated in the sense that $\boldsymbol{q}_{n+1}$ is assumed to be the projection of $\boldsymbol{p}_{n+1}$ and $\boldsymbol{q}_n$ is written as (cf. Figure 116, part b))

$$\boldsymbol{q}_n = \sum_j \varphi_j(\xi^m_{n+1}, \eta^m_{n+1}) \boldsymbol{q_j}_n. \tag{118}$$

Part a) and part b) of the figure are really equivalent, they just represent the same facts from a different point of view. In part a) the projection on the master surface is performed at time t_n, and the differential displacement is calculated at time t_{n+1}, in part b) the projection is done at time t_{n+1} and the differential displacement is calculated at time t_n. Now, the actual position can be written as the sum of the undeformed position and the deformation, i.e. $\boldsymbol{p} = (\boldsymbol{X} + \boldsymbol{v})^s$ and $\boldsymbol{q} = (\boldsymbol{X} + \boldsymbol{v})^m$ leading to:

$$\boldsymbol{s} = (\boldsymbol{X}+\boldsymbol{v})^s_{n+1} - (\boldsymbol{X}+\boldsymbol{v})^m_{n+1}(\xi^m_{n+1}, \eta^m_{n+1}) - (\boldsymbol{X}+\boldsymbol{v})^s_n + (\boldsymbol{X}+\boldsymbol{v})^m_n(\xi^m_{n+1}, \eta^m_{n+1}). \tag{119}$$

Since the undeformed position is no function of time it drops out:

$$\boldsymbol{s} = \boldsymbol{v}^s_{n+1} - \boldsymbol{v}^m_{n+1}(\xi^m_{n+1}, \eta^m_{n+1}) - \boldsymbol{v}^s_n + \boldsymbol{v}^m_n(\xi^m_{n+1}, \eta^m_{n+1}) \tag{120}$$

or:

$$\boldsymbol{s} = \boldsymbol{v}^s_{n+1} - \boldsymbol{v}^m_{n+1}(\xi^m_{n+1}, \eta^m_{n+1}) - \boldsymbol{v}^s_n + \boldsymbol{v}^m_n(\xi^m_n, \eta^m_n) \tag{121}$$

$$+ \boldsymbol{v}^m_n(\xi^m_{n+1}, \eta^m_{n+1}) - \boldsymbol{v}^m_n(\xi^m_n, \eta^m_n) \tag{122}$$

Now, the last two terms are dropped, i.e. it is assumed that the differential deformation at time t_n between positions (ξ^m_n, η^m_n) and $(\xi^m_{n+1}, \eta^m_{n+1})$ is neglegible compared to the differential motion from t_n to t_{n+1}. Then the expression for $\boldsymbol{s}$ simplifies to:

$$\boldsymbol{s} = \boldsymbol{v}^s_{n+1} - \boldsymbol{v}^m_{n+1}(\xi^m_{n+1}, \eta^m_{n+1}) - \boldsymbol{v}^s_n + \boldsymbol{v}^m_n(\xi^m_n, \eta^m_n), \tag{123}$$

and the only quantity to be stored is the difference in deformation between $\boldsymbol{p}$ and $\boldsymbol{q}$ at the actual time and at the time of the beginning of the increment.

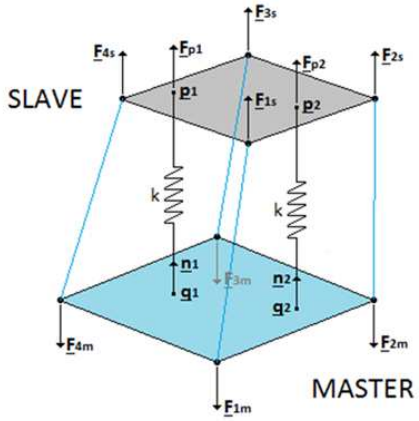


Figure 117: Creation of a face-to-face penalty contact element

6.7.5 Face-to-Face Penalty Contact

General considerations In the face-to-face penalty contact formulation the spring element which was described in the previous section is now applied between an integration point of a slave face and a master face (spring in Figure 117). The contact force at the integration point is subsequently transferred to the nodes of the slave face. This results in contact spring elements connecting a slave face with a master face (full lines in Figure 117). The integration points in the slave faces are not the ordinary Gauss points. Instead, the master and slave mesh are put on top of each other, the common areas, which are polygons (sides of quadratic elements are approximated by piecewise linear lines), are identified and triangulated. For each triangle a 7-node scheme is used (Figure 118). This can result to up to 100 or more integration points within one slave face. It usually leads to a very smooth pressure distribution. Furthermore, it is now irrelevant which side is defined as master and which as slave. In the present formulation the following approximations are used:

- the linear pressure-overclosure relationship is truly bilinear, i.e. zero for positive clearance and linear for penetration (and not quasi bilinear as for node-to-face penalty). The value of c_0 is zero.

- the matching between the slave faces and master faces, the calculation of the resulting integration points and the local normals on the master surface is done once at the start of each increment. This information is not changed while iterating within an increment. The same applies to the calculation of the area for which the slave integration point is representative.

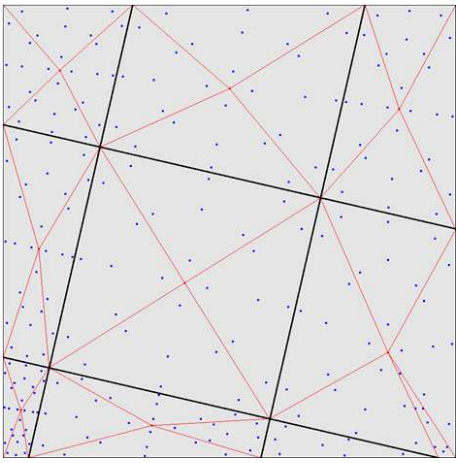


Figure 118: Integration points resulting from the cutting of one master face (big square) with several slave faces (small, slanted squares)

- whether a contact element is active or not is determined in each iteration anew. A contact element is active if the penetration is positive.

Due to the freezing of the match between the slave and master surface within each increment, large deformations of the structure may require small increments.

The contact definition in the input deck is similar to the node-to-face penalty contact except for:

- The contact surfaces (both slave and master) must be face-based.
- On the *CONTACT PAIR card the parameter TYPE=SURFACE TO SURFACE must be specified.
- The SMALL SLIDING parameter on the *CONTACT PAIR card is not allowed.
- The *SURFACE BEHAVIOR card for a linear pressure-overclosure relationship needs only one parameter: the spring constant.
- The *FRICTION card is needed to specify the friction coefficient and the stick slope.

In addition, a new pressure-overclosure relationship is introduced with the name TIED. It can be used to tie surfaces and usually leads to a significantly smoother stress distribution than the MPC's generated by the *TIE option. For the TIED pressure-overclosure relation only two parameters are used: the spring stiffness K (> 0, required), and the stick slope λ (> 0, optional). The friction coefficient is irrelevant.

Weak formulation The contribution of the face-to-face penalty contact to the weak formulation corresponds to the first term on the right hand side of Equation (2.6) in [18], written for both the slave and master side. This amounts to (in the material frame of reference):

$$\int_{A_0^s} \delta(\boldsymbol{U^S} - \boldsymbol{U^M}) \cdot \boldsymbol{T_{(N)}} dA, \tag{124}$$

or, in the spatial frame of reference:

$$\int_{A^s} \delta(\boldsymbol{u^s} - \boldsymbol{u^m}) \cdot \boldsymbol{t_{(n)}} da. \tag{125}$$

Making a Taylor expansion for $\boldsymbol{t_{(n)}}$, which is a function of $\boldsymbol{u_s} - \boldsymbol{u^m}$ and keeping the linear term only (the constant term vanishes since zero differential displacements leads to zero traction) one obtains:

$$\int_{A^s} \delta(\boldsymbol{u^s} - \boldsymbol{u^m}) \cdot \frac{\partial \boldsymbol{t_{(n)}}}{\partial \boldsymbol{u^s}} \cdot (\boldsymbol{u^s} - \boldsymbol{u^m}) da. \tag{126}$$

Notice that the integral is over the slave faces. The corresponding positions on the master side are obtained by local orthogonal projection. The displacements within a face on the slave side can be written as a linear combination of the displacements of the nodes belonging to the face (n_s is the number of nodes belonging to the slave face):

$$\boldsymbol{u^s} = \sum_{i}^{n_s} \varphi_i \boldsymbol{u_i^s}, \tag{127}$$

and similarly for the displacements on the master side (n_m is the number of nodes belonging to the slave face):

$$\boldsymbol{u^m} = \sum_{j}^{n_m} \psi_j \boldsymbol{u_j^m}. \tag{128}$$

Substituting the above expressions in Equation (126) one obtains:

$$\begin{aligned}
&\sum_{f_s} \sum_{i=1}^{n_s} \sum_{j=1}^{n_s} \delta \boldsymbol{u_i^s} \cdot \left[\int_{A_{f_s}} \varphi_i \frac{\partial \boldsymbol{t_{(n)}}}{\partial \boldsymbol{u^s}} \varphi_j da \right] \cdot \boldsymbol{u_j^s} \\
-&\sum_{f_s} \sum_{i=1}^{n_s} \sum_{j=1}^{n_m} \delta \boldsymbol{u_i^s} \cdot \left[\int_{A_{f_s}} \varphi_i \frac{\partial \boldsymbol{t_{(n)}}}{\partial \boldsymbol{u^s}} \psi_j da \right] \cdot \boldsymbol{u_j^m} \\
-&\sum_{f_s} \sum_{i=1}^{n_m} \sum_{j=1}^{n_s} \delta \boldsymbol{u_i^m} \cdot \left[\int_{A_{f_s}} \psi_i \frac{\partial \boldsymbol{t_{(n)}}}{\partial \boldsymbol{u^s}} \varphi_j da \right] \cdot \boldsymbol{u_j^s} \\
+&\sum_{f_s} \sum_{i=1}^{n_m} \sum_{j=1}^{n_m} \delta \boldsymbol{u_i^m} \cdot \left[\int_{A_{f_s}} \psi_i \frac{\partial \boldsymbol{t_{(n)}}}{\partial \boldsymbol{u^s}} \psi_j da \right] \cdot \boldsymbol{u_j^m}.
\end{aligned} \tag{129}$$

"f_s" is one of the faces belonging to the slave surface. This leads to the following stiffness contributions (notice the change in sign, since the weak term has to be transferred to the left hand side of Equation (2.6) in [18]:

$$[K]_{e(iK)(jM)} = -\int_{A_{fs}} \varphi_i \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \varphi_j da, \quad i \in S, j \in S \tag{130}$$

$$[K]_{e(iK)(jM)} = \int_{A_{fs}} \varphi_i \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \psi_j da, \quad i \in S, j \in M \tag{131}$$

$$[K]_{e(iK)(jM)} = \int_{A_{fs}} \psi_i \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \varphi_j da, \quad i \in M, j \in S \tag{132}$$

$$[K]_{e(iK)(jM)} = -\int_{A_{fs}} \psi_i \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \psi_j da, \quad i \in M, j \in M \tag{133}$$

S is the slave face "f_s" at stake, M is the master face to which the orthogonal projection of the infinitesimal slave area da belongs. The integrals in the above expression are evaluated by numerical integration. One could, for instance, use the classical Gauss points in the slave faces. This, however, will not give optimal results, since the master and slave faces do not match and the function to integrate exhibits discontinuities in the derivatives. Much better results are obtained by using the integration scheme presented in the previous section and illustrated in Figure 118. In this way, the above integrals are replaced by:

$$-\int_{A_{fs}} \varphi_i \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \varphi_j da = -\sum_k \varphi_i(\xi_{s_k}, \eta_{s_k}) \varphi_j(\xi_{s_k}, \eta_{s_k}) \left. \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \right|_{\xi_{s_k}, \eta_{s_k}} \|\boldsymbol{J}\|_k w_k, \tag{134}$$

$$\int_{A_{fs}} \varphi_i \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \psi_j da = \sum_k \varphi_i(\xi_{s_k}, \eta_{s_k}) \psi_j(\xi_{m_k}, \eta_{m_k}) \left. \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \right|_{\xi_{s_k}, \eta_{s_k}} \|\boldsymbol{J}\|_k w_k, \tag{135}$$

$$\int_{A_{fs}} \psi_i \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \varphi_j da = \sum_k \psi_i(\xi_{m_k}, \eta_{m_k}) \varphi_j(\xi_{s_k}, \eta_{s_k}) \left. \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \right|_{\xi_{s_k}, \eta_{s_k}} \|\boldsymbol{J}\|_k w_k, \tag{136}$$

$$-\int_{A_{fs}} \psi_i \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \psi_j da = -\sum_k \psi_i(\xi_{m_k}, \eta_{m_k}) \psi_j(\xi_{m_k}, \eta_{m_k}) \left. \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \right|_{\xi_{s_k}, \eta_{s_k}} \|\boldsymbol{J}\|_k w_k, \tag{137}$$

where k is the number of the integration point; (ξ_{s_k}, η_{s_k}) are the local coordinates of the slave integration point; (ξ_{m_k}, η_{m_k}) are the local coordinates of the orthogonal projection of the slave integration point onto the master surface w.r.t. the master face to which the projection belongs; $\|\boldsymbol{J}\|_k$ is the norm of the local Jacobian vector at the integration point on the slave face and w_k is the weight. Notice that the projection of integration points within the same slave face may belong to different master faces. Each slave integration point k leads to a contact element connecting a slave face with a master face and represented by a stiffness matrix of size $3(n_s + n_m)$ x $3(n_s + n_m)$ made up of contributions described by the above equations for just one value of integration point k.

From this one observes that it is sufficient to determine the 3x3 stiffness matrix

$$\left. \frac{\partial \boldsymbol{t_{(n)}}^K}{\partial \boldsymbol{u^s}_M} \right|_{\xi_{s_k}, \eta_{s_k}} \tag{138}$$

at the slave integration points in order to obtain the stiffness matrix of the complete contact element. It represents the derivative of the traction in an integration point of the slave surface with respect to the displacement vector at the same location.

Normal contact stiffness The traction excerted by the master face on the slave face at a slave integration point p can be written analogous to Equation (65):

$$\boldsymbol{t_{(n)}} = f(r)\boldsymbol{n}. \tag{139}$$

For simplicity, in the face-to-face contact formulation it is assumed that within an increment the location (ξ_{m_k}, η_{m_k}) of the projection of the slave integration points on the master face and the local Jacobian on the master face do not change. Consequently (cf. the section 6.7.4):

$$\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{u_p}} = \frac{\partial \xi}{\partial \boldsymbol{u_p}} = \frac{\partial \eta}{\partial \boldsymbol{u_p}} = \boldsymbol{0}. \tag{140}$$

and

$$\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u_p}} = \boldsymbol{I}, \tag{141}$$

which leads to

$$\frac{\partial \boldsymbol{t_{(n)}}}{\partial \boldsymbol{u_p}} = \frac{\partial f}{\partial r} \boldsymbol{n} \otimes \boldsymbol{n}. \tag{142}$$

This is the normal contact contribution to Equation (138).

Tangent contact stiffness Due to the assumption that the projection of the slave integration point on the master surface does not change during and increment, and that the local normal on the master surface does not change either, the equations derived in the section on node-to-face contact simplity to:

$$\frac{\partial \boldsymbol{t}}{\partial \boldsymbol{u_p}} = (\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n}) \cdot \frac{\partial \boldsymbol{s}}{\partial \boldsymbol{u_p}}, \tag{143}$$

where

$$\frac{\partial \boldsymbol{s}}{\partial \boldsymbol{u_p}} = \boldsymbol{I}. \tag{144}$$

Equation (117) now reduces to

$$\begin{aligned}\frac{\partial \boldsymbol{t_{(\tau)}}_{n+1}}{\partial \boldsymbol{u_p}_{n+1}} = \mu \boldsymbol{\xi}_{n+1} \otimes \left[-\boldsymbol{n} \cdot \frac{\partial \boldsymbol{t_{(n)}}_{n+1}}{\partial \boldsymbol{u_p}_{n+1}} \right] \\ + \mu \frac{\| \boldsymbol{t_{(n)}}_{n+1} \|}{\| \boldsymbol{t_{(\tau)}}_{n+1}^{trial} \|} [\boldsymbol{I} - \boldsymbol{\xi}_{n+1} \otimes \boldsymbol{\xi}_{n+1}] \cdot K_t \frac{\partial \boldsymbol{t}_{n+1}}{\partial \boldsymbol{u_p}_{n+1}}.\end{aligned} \tag{145}$$

Be careful to distinguish $\boldsymbol{t_{(n)}}_{n+1}$ and $\boldsymbol{t_{(\tau)}}_{n+1}$, which are tractions, from $\boldsymbol{t}_{n+1}$, which is a tangential differential displacement.

6.8 Materials

A material definition starts with a *MATERIAL key card followed by material specific cards such as *ELASTIC, *EXPANSION, *DENSITY, *HYPERELASTIC, *HYPERFOAM, *DEFORMATION PLASTICITY, *PLASTIC, *CREEP or *USER MATERIAL. To assign a material to an element, the *SOLID SECTION card is used. An element can consist of one material only. Each element in the structure must have a material assigned. Some types of loading require specific material properties: gravity loading requires the density of the material, temperature loading requires the thermal expansion coefficient. A material property can also be required by the type of analysis: a frequency analysis requires the material's density.

Some of the material cards are mutually exclusive, while others are interdependent. Exactly one of the following is required: *ELASTIC, *HYPERELASTIC, *HYPERFOAM, *DEFORMATION PLASTICITY and *USER MATERIAL. The keyword *PLASTIC must be preceded by *ELASTIC(,TYPE=ISO). The same applies to the *CREEP card. A *PLASTIC card in between the *ELASTIC and *CREEP card defines a viscoplastic material. The other keywords can be used according to your needs.

If any of the materials defined in the input deck is not a linear elastic material, geometric nonlinearities are automatically taken into account (i.e. NLGEOM is activated). This does not apply to user-defined materials: here the user can switch between geometric linear and geometric nonlinear calculations by omitting or including the NLGEOM parameter on the *STEP card.

6.8.1 Linear elastic materials

Linear elastic materials are characterized by an elastic potential of which only the quadratic terms in the strain are kept. It can be defined in a isotropic, orthotropic or fully anisotropic version. Isotropic linear elastic materials are characterized by their Young's modulus and Poisson's coefficient. Common steels are usually isotropic. Orthotropic materials, such as wood or cubic single crystals are characterized by 9 nonzero constants and fully anisotropic materials by 21 constants. For elastic materials the keyword *ELASTIC is used.

6.8.2 Linear elastic materials for large strains (Ciarlet model)

In [18] it is explained that substituting the infinitesimal strains in the classical Hooke law by the Lagrangian strain and the stress by the Piola-Kirchoff stress of the second kind does not lead to a physically sensible material law. In particular, such a model (also called St-Venant-Kirchoff material) does not exhibit large stresses when compressing the volume of the material to nearly zero. An alternative is the following stored-energy function developed by Ciarlet [17]:

$$\Sigma = \frac{\lambda}{4}(III_C - \ln III_C - 1) + \frac{\mu}{4}(I_C - \ln III_C - 3). \tag{146}$$

The stress-strain relation amounts to ($\boldsymbol{S}$ is the Piola-Kirchoff stress of the second kind) :

$$\boldsymbol{S} = \frac{\lambda}{2}(\det\boldsymbol{C} - 1)\boldsymbol{C^{-1}} + \mu(\boldsymbol{I} - \boldsymbol{C^{-1}}), \tag{147}$$

and the derivative of $\boldsymbol{S}$ with respect to the Green tensor $\boldsymbol{E}$ reads (component notation):

$$\frac{dS^{IJ}}{dE_{KL}} = \lambda(\det\boldsymbol{C})C^{-1^{KL}}C^{-1^{IJ}} + [2\mu - \lambda(\det\boldsymbol{C} - 1)]C^{-1^{IK}}C^{-1^{LJ}}. \tag{148}$$

This model was implemented into CalculiX by Sven Kaßbohm. The definition consists of a *MATERIAL card defining the name of the material. This name HAS TO START WITH "CIARLET_EL" but can be up to 80 characters long. Thus, the last 70 characters can be freely chosen by the user. Within the material definition a *USER MATERIAL card has to be used satisfying:

First line:

- *USER MATERIAL

- Enter the CONSTANTS parameter and its value, i.e. 2.

Following line:

- λ.
- μ.
- Temperature.

Repeat this line if needed to define complete temperature dependence.
For this model, there are no internal state variables.

`Example:`

```
*MATERIAL,NAME=CIARLET_EL
*USER MATERIAL,CONSTANTS=2
80769.23,121153.85,400.
```

defines a single crystal with elastic constants λ=121153.85 and μ=80769.23 for a temperature of 400. Recall that

$$\mu = \frac{E}{2(1+\nu)} \tag{149}$$

and

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}, \tag{150}$$

where E is Young's modulus and ν is Poisson's coefficient.

6.8.3 Ideal gas for quasi-static calculations

A special case of a linear elastic isotropic material is an ideal gas for small pressure deviations. From the ideal gas equation one finds that the pressure deviation dp is related to a density change $d\rho$ by

$$dp = \frac{d\rho}{\rho_0}\rho_0 rT, \tag{151}$$

where ρ_0 is the density at rest, r is the specific gas constant and T is the temperature in Kelvin. From this one can derive the equations

$$t_{11} = t_{22} = t_{33} = (\epsilon_{11} + \epsilon_{22} + \epsilon_{33})\rho_0 rT \tag{152}$$

and

$$t_{12} = t_{13} = t_{23} = 0, \tag{153}$$

where $\boldsymbol{t}$ denotes the stress and $\boldsymbol{\epsilon}$ the linear strain. This means that an ideal gas can be modeled as an isotropic elastic material with Lamé constants $\lambda = \rho_0 rT$ and $\mu = 0$. This corresponds to a Young's modulus $E = 0$ and a Poisson coefficient $\nu = 0.5$. Since the latter values lead to numerical difficulties it is advantageous to define the ideal gas as an orthotropic material with $D_{1111} = D_{2222} = D_{3333} = D_{1122} = D_{1133} = D_{2233} = \lambda$ and $D_{1212} = D_{1313} = D_{2323} = 0$.

6.8.4 Hyperelastic and hyperfoam materials

Hyperelastic materials are materials for which a potential function exists such that the second Piola-Kirchhoff stress tensor can be written as the derivative of this potential with respect to the Lagrangian strain tensor. This definition includes linear elastic materials, although the term hyperelastic material is usually reserved for proper nonlinear elastic materials. One important class constitutes the isotropic hyperelastic materials, for which the potential function is a function of the strain invariants only. All rubber material models presently included in CalculiX are of that type (Arruda-Boyce, Mooney-Rivlin, Neo Hooke, Ogden, Polynomial, Reduced Polynomial and Yeoh). They are selected by the keyword *HYPERELASTIC. Rubber materials are virtually incompressible (virtually no dependence on the third Lagrangian strain invariant which takes values close to 1). The dependence on the third invariant (the compressibility) is separated from the dependence on the first two invariants and is governed by so called compressibility coefficients, taking the value 0 for perfectly incompressible materials. Perfectly incompressible materials require the use of hybrid finite elements, in which the pressure is taken as an additional independent variable (in addition to the displacements). CalculiX does not provide such elements. Consequently, a slight amount of compressibility is required for CalculiX to work. If the user inserts zero compressibility coefficients, CalculiX uses a default value corresponding to an initial value of the Poisson coefficient of 0.475.

Another example of isotropic hyperelastic materials are the hyperfoam materials, which are also implemented in CalculiX (activated by the keyword *HYPERFOAM). Hyperfoam materials are very compressible.

Other materials frequently simulated by a hyperelastic model are human tissue (lung tissue, heart tissue..). To simulate these classes of materials anisotropic hyperelastic models are used, in which the potential function depends on the Lagrangian strain tensor components. No such models are implemented in CalculiX, although their inclusion is not difficult to manage. For further information the reader is referred to [8]. A very nice treatment of the large deformation theory for hyperelastic materials is given in [67].

6.8.5 Deformation plasticity

Deformation plasticity is characterized by a one-to-one (bijective) relationship between the strain and the stress. This relationship is a three-dimensional generalization of the one-dimensional Ramberg-Osgood law frequently used for metallic materials (e.g. in the simple tension test) yielding a monotonic increas-

ing function of the stress as a function of the strain. Therefore, deformation plasticity is very well suited to model the relation between the Cauchy (true) stress and the strain. Because tensile and compressive test results coincide well when plotting the Cauchy stress versus the logarithmic strain (soon to be defined), these quantities are generally used in the deformation plasticity law. The implementation in CalculiX (keyword card *DEFORMATION PLASTICITY), however, uses the relationship to model the dependence of the Cauchy (true) stress on the Eulerian strain. For all practical purposes, the Eulerian strain coincides with the logarithmic strain. For a tensile test specimen, with initial length L, initial cross section A_0, final length $L + \Delta L$ and final cross section A, loaded by a force F, the Cauchy stress σ, the logarithmic strain ϵ_{log} and the Eulerian strain ϵ_{Euler} satisfy:

$$\sigma = F/A = \frac{F(L + \Delta L)}{A_0 L} \tag{154}$$

$$\epsilon_{log} = ln \left[1 + \frac{\Delta L}{L}\right] \tag{155}$$

$$\epsilon_{Euler} = \frac{\Delta L}{L} \left[1 - \frac{\Delta L}{2L}\right] \tag{156}$$

The difference between the logarithmic strain and the Eulerian strain is about 1.3 % for an Engineering strain $\Delta L/L = 20\%$. The user should give the Ramberg-Osgood material constants directly (by plotting a Cauchy stress versus Eulerian strain curve and performing a fit).

6.8.6 Incremental (visco)plasticity

The implementation of incremental plasticity in CalculiX follows the algorithms in [68] and [69] and is based on the notion of an intermediate stress-free configuration. The deformation is viewed as a plastic flow due to dislocation motion followed by elastic stretching and rotation of the crystal lattice. This is synthesized by a local multiplicative decomposition of the deformation gradient $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$ where $F_{kK} = x_{k,K}$ in Cartesian coordinates.

In the present implementation, the elastic response is isotropic and is deduced from a stored-energy function (hyperelastic response). Furthermore, the plastic flow is isochoric (the volume is conserved) and the classical von Mises-Huber yield condition applies. This condition can be visualized as a sphere in principal deviatoric stress space.

The hardening can consist of isotropic hardening, resulting in an expansion or contraction of the yield surface, of kinematic hardening, resulting in a translation of the yield surface, or of a combination of both. The hardening curve should yield the von Mises true stress versus the equivalent plastic logarithmic strain (cf. deformation plasticity for its definition).

Incremental plasticity is defined by the *PLASTIC card, followed by the isotropic hardening curve for isotropic hardening or the kinematic hardening

curve for kinematic and combined hardening. For combined hardening, the isotropic hardening curve is defined by the *CYCLIC HARDENING card. The *PLASTIC card should be preceded within the same material definition by an *ELASTIC card, defining the isotropic elastic properties of the material.

By allowing the stress to leave the yield surface temporarily in order to regain it with time, creep effects can be modeled [66]. The viscous part of the viscoplastic law is defined by the *CREEP card. Default is a Norton type law. However, the user can also define his own law in user subroutine creep.f. If the *CREEP card is not preceded by a *PLASTIC card, a zero yield surface without any hardening effects is assumed. The *CREEP card must be preceded by an *ELASTIC card defining the isotropic elastic properties of the material. Notice that creep behavior is switched off in a *STATIC step.

For this model, there are 13 internal state variables:

- the accumulated equivalent plastic strain $\bar{e^p}$ (1)
- the unit tensor minus the inverse plastic right Cauchy-Green tensor and divided by two $(\mathbf{I}-\mathbf{C^{p^{-1}}})/2$. For small deformations the resulting tensor coincides with the infinitesimal plastic strain tensor $\epsilon^{\mathbf{P}}$ (6)
- the back stress $\mathbf{\Gamma}$ (6)

These variables are accessible through the *EL PRINT (.dat file) and *EL FILE (.frd file) keywords in exactly this order (label SDV).

By using the *CHANGE MATERIAL, *CHANGE PLASTIC, *STATIC and *VISCO cards the user can switch between a purely plastic and creep behavior. The viscoplastic model implemented in CalculiX is an overstress model, i.e. creep only occurs above the yield stress. For a lot of materials this is not realistic. At high temperatures creep is frequently observed well below the yield stress. To simulate this behavior one can set the yield stress to zero. In order to simulate an initial large plastic deformation (e.g. due to forging or other machining operations) followed by creep at high temperature at operation conditions one can proceed as follows: one defines the material as a viscoplastic material using the *PLASTIC and *CREEP card. To switch off the creep behavior in the machining step one uses the *STATIC procedure. In a subsequent step at operating conditions the viscous behavior is switched on using the *VISCO procedure whereas the yield stress is set to zero by means of a *CHANGE MATERIAL and *CHANGE PLASTIC card.

6.8.7 Tension-only and compression-only materials.

These are material models which can be used to simulate textile behavior (tension-only) and concrete (compression-only). In essence, a one-dimensional Hooke-type relationship is established between the principal stresses and principal strains, thereby suppressing the compressive stress range (tension-only materials) or tensile stress range (compression-only materials).

The Cauchy-Green tensor can be written as a function of its eigenvalues and eigenvectors as follows:

$$\mathbf{C} = \sum_{i=1}^{3} \Lambda_i \mathbf{M^i}, \tag{157}$$

where $\mathbf{M^i}$ are the structural tensors satisfying $\mathbf{M^i} = \mathbf{N_i} \otimes \mathbf{N^i}$, $\mathbf{N^i}$ being the principal directions [18]. From this, the second Piola-Kirchhoff stress tensor can be defined by:

$$\mathbf{S} = \sum_{i=1}^{3} f(\Lambda_i) \mathbf{M^i}, \tag{158}$$

where, for tension-only materials,

$$f(\Lambda_i) = E \left(\frac{\Lambda_i - 1}{2} \right) \left[\frac{1}{2} + \frac{1}{\pi} \tan^{-1} \left(\frac{\Lambda_i - 1}{2\epsilon} \right) \right], \tag{159}$$

where E is an elastic modulus, the term within the first parentheses is a Lagrange principal strain and the term within the square brackets is a correction term suppressing the negative stresses (pressure). It is a function tending to zero for negative strains (-0.5 being the smallest possible Lagrange strain), to one for large positive strains and switches between both in a region surrounding zero strain. The extent of this region is controlled by the parameter ϵ: the smaller its value, the smaller the transition region (the sharper the switch). It is a monotonically increasing function of the strain, thus guaranteeing convergence. The correction term is in fact identical to the term used to cut off tensile stresses for penalty contact in Equation(59) and Figure (114). Replacing "overclosure" and "pressure" by "principal strain" and "principal stress" in that figure yields the function f. Although compressive stresses are suppressed, they are not zero altogether. The maximum allowed compressive stress (in absolute value) amounts to $E\epsilon/\pi$. Instead of chosing E and ϵ the user defines E and the maximum allowed compressive stress, from which ϵ is determined.

The material definition consists of a *MATERIAL card defining the name of the material. This name HAS TO START WITH "TENSION_ONLY" but can be up to 80 characters long. Thus, the last 68 characters can be freely chosen by the user. Within the material definition a *USER MATERIAL card has to be used satisfying:

First line:

- *USER MATERIAL
- Enter the CONSTANTS parameter and its value. The value of this parameter is 2.

Following line:

- E.

- absolute value of the maximum allowed pressure.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

For a compression-only materials the name of the material has to start with "COMPRESSION_ONLY" (maximum 64 characters left to be chosen by the user) and the second constant is the maximum allowed tension. Examples are leifer2 and concretebeam in the test example suite.

6.8.8 Fiber reinforced materials.

This is a model which was conceived by G. Holzapfel et al. [30] to model arterial walls. It is an anisotropic hyperelastic model, consisting of an isotropic neo-Hooke potential for the base material, complemented by exponential strenghtening terms in fiber direction. The mathematical form of the potential satisfies:

$$U = C_{10}(\bar{I}_1 - 3) + \frac{1}{D_1}(J-1)^2 + \sum_{i=1}^{n} \frac{k_{1i}}{2k_{2i}} \left[e^{k_{2i}\langle \bar{J}_{4i} - 1 \rangle^2} - 1 \right] \tag{160}$$

where $\langle x \rangle = 0$ for $x < 0$ and $\langle x \rangle = x$ for $x \geq 0$. Thus, the fibers do not take up any force under compression. Although the material was originally defined for arteries, it is expected to work well for other fiber reinforced materials too, such as reinforced nylon. The material model implemented thus far can cope with up to 4 different fibers. The material definition consists of a *MATERIAL card defining the name of the material. This name HAS TO START WITH "ELASTIC_FIBER" but can be up to 80 characters long. Thus, the last 67 characters can be freely chosen by the user. Within the material definition a *USER MATERIAL card has to be used satisfying:

First line:

- *USER MATERIAL
- Enter the CONSTANTS parameter and its value. The value of this parameter is 2+4n, where n is the number of fiber directions.

Following line if one fiber direction is selected:

- C_{10}.
- D_1.
- n_{x1}: x-direction cosine of fiber direction.
- n_{y1}: y-direction cosine of fiber direction.
- k_{11}.
- k_{21}.

- Temperature.

Repeat this line if needed to define complete temperature dependence. The z-direction cosine of the fiber direction is determined from the x- and y-direction cosine since the direction norm is one. If a local axis system is defined for an element consisting of this material (with *ORIENTATION)the direction cosines are defined in the local system.

If more than one fiber direction is selected (up to a maximum of four), the four entries characterizing fiber direction 1 are repeated for the subsequent directions. Per line no more than eight entries are allowed. If more are needed, continue on the next line.

Example:

```
*MATERIAL,NAME=ELASTIC_FIBER
*USER MATERIAL,CONSTANTS=18
1.92505,0.026,0.,0.7071,2.3632,0.8393,0,-0.7071,
2.3632,0.8393,0.7071,0.,2.3632,0.8393,-0.7071,0.,
2.3632,0.8393
```

defines an elastic fiber materials with four different fiber directions (0,0.7071,0.7071), (0,-0.7071,0.7071), (0.7071,0.,0.7071) and (-0.7071,0.,0.7071). The constants are $C_{10} = 1.92505,\ D_1 = 0.026$ and $k_{1i} = 2.3632,\ k_{2i} = 0.8393\ \forall\ i\ \in\ \{1, 2, 3, 4\}$.

6.8.9 The Cailletaud single crystal model.

The single crystal model of Georges Cailletaud and co-workers [49][50] describes infinitesimal viscoplasticity in metallic components consisting of one single crystal. The orientations of the slip planes and slip directions in these planes is generally known and described by the normal vectors $\mathbf{n}^\beta$ and direction vectors $\mathbf{l}^\beta$, respectively, where β denotes one of slip plane/slip direction combinations. The slip planes and slip directions are reformulated in the form of a slip orientation tensor $\mathbf{m}^\beta$ satisfying:

$$\mathbf{m}^\beta = (\mathbf{n}^\beta \otimes \mathbf{l}^\beta + \mathbf{l}^\beta \otimes \mathbf{n}^\beta)/2. \tag{161}$$

The total strain is supposed to be the sum of the elastic strain and the plastic strain:

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^{\boldsymbol{e}} + \boldsymbol{\epsilon}^{\boldsymbol{p}}. \tag{162}$$

In each slip plane an isotropic hardening variable q_1 and a kinematic hardening variable q_2 are introduced representing the isotropic and kinematic change of the yield surface, respectively. The yield surface for orientation β takes the form:

$$h^\beta := \left|\boldsymbol{\sigma} : \mathbf{m}^\beta + q_2^\beta\right| - r_0^\beta + \sum_{\alpha=1}^{n^\beta} H_{\beta\alpha} q_1^\alpha = 0 \tag{163}$$

where n^β is the number of slip orientations for the material at stake, $\boldsymbol{\sigma}$ is the stress tensor, r_0^β is the size of the elastic range at zero yield and $H_{\beta\alpha}$ is a matrix of interaction coefficients. The constitutive equations for the hardening variables satisfy:

$$q_1^\beta = -b^\beta Q^\beta \alpha_1^\beta \tag{164}$$

and

$$q_2^\beta = -c^\beta \alpha_2^\beta \tag{165}$$

where α_1^β and α_2^β are the hardening variables in strain space. The constitutive equation for the stress is Hooke's law:

$$\boldsymbol{\sigma} = \boldsymbol{C} : \boldsymbol{\epsilon^e}. \tag{166}$$

The evolution equations for the plastic strain and the hardening variables in strain space are given by:

$$\dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}} = \sum_{\beta=1}^{n^\beta} \dot{\gamma}^\beta \mathbf{m}^\beta sgn(\boldsymbol{\sigma} : \mathbf{m}^\beta + q_2^\beta), \tag{167}$$

$$\dot{\alpha}_1^\beta = \dot{\gamma}^\beta \left(1 + \frac{q_1^\beta}{Q^\beta}\right) \tag{168}$$

and

$$\dot{\alpha}_2^\beta = \dot{\gamma}^\beta \left[\varphi^\beta sgn(\boldsymbol{\sigma} : \mathbf{m}^\beta + q_2^\beta) + \frac{d^\beta q_2^\beta}{c^\beta}\right]. \tag{169}$$

The variable $\dot{\gamma}^\beta$ is the consistency coefficient known from the Kuhn-Tucker conditions in optimization theory [44]. It can be proven to satisfy:

$$\dot{\gamma}^\beta = \left|\dot{\epsilon}^{p^\beta}\right|, \tag{170}$$

where $\dot{\epsilon}^{p^\beta}$ is the flow rate along orientation β. The plastic strain rate is linked to the flow rate along the different orientations by

$$\dot{\boldsymbol{\epsilon}}^{\boldsymbol{p}} = \sum_{\beta=1}^{n^\beta} \dot{\epsilon}^{p^\beta} \mathbf{m}^\beta. \tag{171}$$

The parameter φ^β in equation (169) is a function of the accumulated shear flow in absolute value through:

$$\varphi^\beta = \phi^\beta + (1 - \phi^\beta) e^{-\delta^\beta \int_0^t \dot{\gamma}^\beta dt} \tag{172}$$

Finally, in the Cailletaud model the creep rate is a power law function of the yield exceedance:

$$\dot{\gamma}^{\beta} = \left\langle \frac{h^{\beta}}{K^{\beta}} \right\rangle^{n^{\beta}} . \tag{173}$$

The brackets $\langle\rangle$ reduce negative function values to zero while leaving positive values unchanged, i.e. $\langle x\rangle = 0$ if $x < 0$ and $\langle x\rangle = x$ if $x \geq 0$.

In the present umat routine, the Cailletaud model is implemented for a Nickel base single crystal. It has two slip systems, a octaeder slip system with three slip directions $< 011 >$ in four slip planes $\{111\}$, and a cubic slip system with two slip directions $< 011 >$ in three slip planes $\{001\}$. The constants for all octaeder slip orientations are assumed to be identical, the same applies for the cubic slip orientations. Furthermore, there are three elastic constants for this material. Consequently, for each temperature 21 constants need to be defined: the elastic constants C_{1111}, C_{1122} and C_{1212}, and a set $\{K^{\beta}, n^{\beta}, c^{\beta}, d^{\beta}, \phi^{\beta}, \delta^{\beta}, r_0^{\beta}, Q^{\beta}, b^{\beta}\}$ per slip system. Apart from these constants 18^2 interaction coefficients need to be defined. These are taken from the references [49][50] and assumed to be constant. Their values are included in the routine and cannot be influence by the user through the input deck.

The material definition consists of a *MATERIAL card defining the name of the material. This name HAS TO START WITH "SINGLE_CRYSTAL" but can be up to 80 characters long. Thus, the last 66 characters can be freely chosen by the user. Within the material definition a *USER MATERIAL card has to be used satisfying:

First line:

- *USER MATERIAL
- Enter the CONSTANTS parameter and its value, i.e. 21.

Following lines, in sets of 3:

First line of set:

- C_{1111}.
- C_{1122}.
- C_{1212}.
- K^{β} (octaeder slip system).
- n^{β} (octaeder slip system).
- c^{β} (octaeder slip system).
- d^{β} (octaeder slip system).
- ϕ^{β} (octaeder slip system).

Second line of set:

- δ^β (octaeder slip system).
- r_0^β (octaeder slip system).
- Q^β (octaeder slip system).
- b^β (octaeder slip system).
- K^β (cubic slip system).
- n^β (cubic slip system).
- c^β (cubic slip system).
- d^β (cubic slip system).

Third line of set:

- ϕ^β (cubic slip system).
- δ^β (cubic slip system).
- r_0^β (cubic slip system).
- Q^β (cubic slip system).
- b^β (cubic slip system).
- Temperature.

Repeat this set if needed to define complete temperature dependence.

The crystal principal axes are assumed to coincide with the global coordinate system. If this is not the case, use an *ORIENTATION card to define a local system.

For this model, there are 60 internal state variables:

- the plastic strain tensor $\boldsymbol{\epsilon^p}$ (6)
- the isotropic hardening variables q_1^β (18)
- the kinematic hardening variables q_2^β (18)
- the accumulated absolute value of the slip rate $\int_0^t \dot{\gamma^\beta} dt$ (18)

These variables are accessible through the *EL PRINT (.dat file) and *EL FILE (.frd file) keywords in exactly this order (label SDV). The *DEPVAR card must be included in the material definition with a value of 60.

```
Example:

*MATERIAL,NAME=SINGLE_CRYSTAL
*USER MATERIAL,CONSTANTS=21
135468.,68655.,201207.,1550.,3.89,18.E4,1500.,1.5,
100.,80.,-80.,500.,980.,3.89,9.E4,1500.,
2.,100.,70.,-50.,400.
*DEPVAR
60
```

defines a single crystal with elastic constants $\{135468., 68655., 201207.\}$, octaeder parameters $\{1550., 3.89, 18.E4, 1500., 1.5, 100., 80., -80., 500.\}$ and cubic parameters $\{980., 3.89, 9.E4, 1500., 2., 100., 70., -50.\}$ for a temperature of 400.

6.8.10 The Cailletaud single crystal creep model.

This is the Cailletaud single crystal model reduced to the creep case, i.e. the yield surface is reduced to zero.

The material definition consists of a *MATERIAL card defining the name of the material. This name HAS TO START WITH "SINGLE_CRYSTAL_CREEP" but can be up to 80 characters long. Thus, the last 60 characters can be freely chosen by the user. Within the material definition a *USER MATERIAL card has to be used satisfying:

First line:

- *USER MATERIAL
- Enter the CONSTANTS parameter and its value, i.e. 7.

Following line:

- C_{1111}.
- C_{1122}.
- C_{1212}.
- K^{β} (octaeder slip system).
- n^{β} (octaeder slip system).
- K^{β} (cubic slip system).
- n^{β} (cubic slip system).
- Temperature.

Repeat this line if needed to define complete temperature dependence.

The crystal principal axes are assumed to coincide with the global coordinate system. If this is not the case, use an *ORIENTATION card to define a local system.

For this model, there are 24 internal state variables:

- the plastic strain tensor $\boldsymbol{\epsilon^p}$ (6)
- the accumulated absolute value of the slip rate $\int_0^t \dot{\gamma^\beta} dt$ (18)

These variables are accessible through the *EL PRINT (.dat file) and *EL FILE (.frd file) keywords in exactly this order (label SDV). The *DEPVAR card must be included in the material definition with a value of 24.

Example:

```
*MATERIAL,NAME=SINGLE_CRYSTAL
*USER MATERIAL,CONSTANTS=21
135468.,68655.,201207.,1550.,3.89,980.,3.89,400.
*DEPVAR
24
```

defines a single crystal with elastic constants $\{135468., 68655., 201207.\}$, octaeder parameters $\{1550., 3.89\}$ and cubic parameters $\{980., 3.89\}$ for a temperature of 400.

6.8.11 Elastic anisotropy with isotropic viscoplasticity.

This model describes small deformations for elastically anisotropic materials with a von Mises type yield surface. Often, this model is used as a compromise for anisotropic materials with lack of data or detailed knowledge about the anisotropic behavior in the viscoplastic range.

The total strain is supposed to be the sum of the elastic strain and the plastic strain:

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon^e} + \boldsymbol{\epsilon^p}. \tag{174}$$

An isotropic hardening variable q_1 and a kinematic hardening tensor $\mathbf{q_2}$ are introduced representing the isotropic and kinematic change of the yield surface, respectively. The yield surface takes the form:

$$f := \|\boldsymbol{dev(\sigma)} + \mathbf{q_2}\| + \sqrt{\frac{2}{3}}(q_1 - r_0) = 0 \tag{175}$$

where $\boldsymbol{dev(\sigma)}$ is the deviatoric stress tensor, and r_0 is the size of the elastic range at zero yield. The constitutive equations for the hardening variables satisfy:

$$q_1 = -d_1\alpha_1 \tag{176}$$

and

$$\mathbf{q_2} = -\frac{2}{3} d_2 \boldsymbol{\alpha_2} \tag{177}$$

where α_1 and $\boldsymbol{\alpha_2}$ are the hardening variables in strain space. It can be shown that

$$\alpha_1 = \epsilon^{peq}, \tag{178}$$

$$\alpha_2{}^{eq} = \epsilon^{peq}, \tag{179}$$

where ϵ^{peq} is the equivalent plastic strain defined by

$$\epsilon^{peq} = \sqrt{\frac{2}{3}} \left\| \boldsymbol{\epsilon^p} \right\|. \tag{180}$$

and $\alpha_2{}^{eq}$ is the equivalent value of the tensor $\boldsymbol{\alpha_2}$ defined in a similar way. Thus, the constitutive equations amount to

$$q_1 = -d_1 \epsilon^{peq} \tag{181}$$

and

$$q_2{}^{eq} = d_2 \epsilon^{peq}, \tag{182}$$

where

$$q_2{}^{eq} = \sqrt{\frac{3}{2}} \left\| \mathbf{q_2} \right\| \tag{183}$$

has the meaning of an equivalent stress value or von Mises value. The same applies to q_1. Consequently, the constitutive equations assume a linear relationship between the hardening stress and the equivalent plastic strain.

The constitutive equation for the stress is Hooke's law:

$$\boldsymbol{\sigma = C : \epsilon^e}. \tag{184}$$

The evolution equations for the plastic strain and the hardening variables in strain space are given by:

$$\boldsymbol{\dot{\epsilon}^p} = \dot{\gamma} \mathbf{n}, \tag{185}$$

$$\dot{\alpha}_1 = \sqrt{\frac{2}{3}} \dot{\gamma}, \tag{186}$$

and

$$\boldsymbol{\dot{\alpha}_2} = \dot{\gamma} \mathbf{n}, \tag{187}$$

where

$$\mathbf{n} = \frac{\boldsymbol{dev}(\boldsymbol{\sigma}) + \mathbf{q_2}}{\|\boldsymbol{dev}(\boldsymbol{\sigma}) + \mathbf{q_2}\|}. \tag{188}$$

The variable $\dot{\gamma}$ is the consistency coefficient known from the Kuhn-Tucker conditions in optimization theory [44]. It can be proven to satisfy:

$$\dot{\gamma} = \sqrt{\frac{3}{2}}\dot{\epsilon}^{peq}, \tag{189}$$

Finally, the creep rate is modeled as a power law function of the yield exceedance and total time t:

$$\dot{\epsilon^{peq}} = A \left\langle \sqrt{\frac{3}{2}} f \right\rangle^n t^m. \tag{190}$$

The brackets $\langle\rangle$ reduce negative function values to zero while leaving positive values unchanged, i.e. $\langle x\rangle = 0$ if $x < 0$ and $\langle x\rangle = x$ if $x \geq 0$.

In the present implementation orthotropic elastic behavior is assumed. Consequently, for each temperature 15 constants need to be defined: the elastic constants C_{1111}, C_{1122}, C_{2222},C_{1133}, C_{2233}, C_{3333},C_{1212}, C_{1313}, C_{2323}, and the viscoplastic constants r_0, d_1, d_2, A, n, m.

The material definition consists of a *MATERIAL card defining the name of the material. This name HAS TO START WITH "ANISO_PLAS" but can be up to 80 characters long. Thus, the last 70 characters can be freely chosen by the user. Within the material definition a *USER MATERIAL card has to be used satisfying:

First line:

- *USER MATERIAL
- Enter the CONSTANTS parameter and its value, i.e. 15.

Following lines, in sets of 2:

First line of set:

- C_{1111}.
- C_{1122}.
- C_{2222}.
- C_{1133}.
- C_{2233}.
- C_{3333}.
- C_{1212}.

- C_{1313}.

Second line of set:

- C_{2323}.
- r_0.
- d_1.
- d_2.
- A.
- n.
- m.
- Temperature.

Repeat this set if needed to define complete temperature dependence.

The principal axes of the material are assumed to coincide with the global coordinate system. If this is not the case, use an *ORIENTATION card to define a local system.

For this model, there are 14 internal state variables:

- the equivalent plastic strain ϵ^{peq} (1)
- the plastic strain tensor $\boldsymbol{\epsilon^p}$ (6)
- the isotropic hardening variable α_1 (1)
- the kinematic hardening tensor $\alpha_{\mathbf{2}}$ (6)

These variables are accessible through the *EL PRINT (.dat file) and *EL FILE (.frd file) keywords in exactly this order (label SDV). The *DEPVAR card must be included in the material definition with a value of 14.

```
Example:

*MATERIAL,NAME=ANISO_PLAS
*USER MATERIAL,CONSTANTS=15
500000.,157200.,500000.,157200.,157200.,500000.,126200.,126200.,
126200.,0.,0.,0.,1.E-10,5,0.
*DEPVAR
14
```

defines a single crystal with elastic constants 500000., 157200., 500000., 157200., 157200., 500000., 126200., 126200., 126200., and viscoplastic parameters $r_0 = 0.$, $d_1 = 0.$, $d_2 = 0.$, $A = 10^{-10}$, $n = 5$ and $m = 0$. Thus, the yield surface has a zero radius and there is no hardening. Only creep is activated.

6.8.12 User materials

Other material laws can be defined by the user by means of the *USER MATERIAL keyword card. More information and examples can be found in section 8.5.

6.9 Types of analysis

An analysis type applies to a complete step, which starts with a *STEP card and ends with an *END STEP card. The analysis type, the loading and field output requests must be defined in between.

6.9.1 Static analysis

In a static analysis the time dimension is not involved. The loading is assumed to be applied in a quasi-static way, i.e. so slow that inertia effects can be neglected. A static analysis is defined by the key word *STATIC. A static step can be geometrically linear or nonlinear. In both cases a Lagrangian point of view is taken and all variables are specified in the material frame of reference [20]. Thus, the stress used internally in CalculiX is the second Piola-Kirchhoff tensor acting on the undeformed surfaces.

For geometrically linear calculations the infinitesimal strains are taken (linearized version of the Lagrangian strain tensor), and the loads do not interfere with each other. Thus, the deformation due to two different loads is the sum of the deformation due to each of them. For linear calculations the difference between the Cauchy and Piola-Kirchhoff stresses is neglected.

For geometrically nonlinear calculations, the full Lagrangian strain tensor is used. A geometrically nonlinear calculation is triggered by the parameter NLGEOM on the *STEP card. It is also automatically triggered (whether the parameter NLGEOM is used or not) by nonlinear material behavior (e.g. *HYPERELASTIC, *PLASTIC.., but NOT for *USER MATERIAL). The step is usually divided into increments, and the user is supposed to provide an initial increment length and the total step length on the *STATIC card. The increment length can be fixed (parameter DIRECT on the *STATIC card) or automatic. In case of automatic incrementation, the increment length is automatically adjusted according to the convergence characteristics of the problem. In each increment, the program iterates till convergence is reached, or a new attempt is made with a smaller increment size. In each iteration the geometrically linear stiffness matrix is augmented with an initial displacement stiffness due to the deformation in the last iteration and with an initial stress stiffness due to the last iteration's stresses [78]. For the output on file the second Piola-Kirchhoff stress is converted into the Cauchy or true stress, since this is the stress which is really acting on the structure.

Special provisions are made for cyclic symmetric structures. A cyclic symmetric structure is characterized by N identical sectors, see Figure 119 and the discussion in next section. Static calculations for such structures under cyclic symmetric loading lead to cyclic symmetric displacements. Such calculations

can be reduced to the consideration of just one sector, the so-called datum sector, subject to cyclic symmetry conditions, i.e. the right boundary of the sector exhibits the same displacements as the left boundary, in cylindrical coordinates (NOT in rectangular coordinates!). The application of these boundary conditions is greatly simplified by the use of the keyword cards *SURFACE, *TIE and *CYCLIC SYMMETRY MODEL, defining the nodes on left and right boundary and the sector size. Then, the appropriate multiple point constraints are generated automatically. This can also be used for a static preload step prior to a perturbative frequency analysis.

6.9.2 Frequency analysis

In a frequency analysis the lowest eigenfrequencies and eigenmodes of the structure are calculated. In CalculiX, the mass matrix is not lumped, and thus a generalized eigenvalue problem has to be solved. The theory can be found in any textbook on vibrations or on finite elements, e.g. [78]. A crucial point in the present implementation is that, instead of looking for the smallest eigenfrequencies of the generalized eigenvalue problem, the largest eigenvalues of the inverse problem are determined. For large problems this results in execution times cut by about a factor of 100 (!). The inversion is performed by calling the linear equation solver SPOOLES. A frequency step is triggered by the key word *FREQUENCY and can be perturbative or not.

If the perturbation parameter is not activated on the *STEP card, the frequency analysis is performed on the unloaded structure, constrained by the homogeneous SPC's and MPC's. Any steps preceding the frequency step do not have any influence on the results.

If the perturbation parameter is activated, the stiffness matrix is augmented by contributions resulting from the displacements and stresses at the end of the last non-perturbative static step, if any, and the material parameters are based on the temperature at the end of that step. Thus, the effect of the centrifugal force on the frequencies in a turbine blade can be analyzed by first performing a static calculation with these loads, and selecting the perturbation parameter on the *STEP card in the subsequent frequency step. The loading at the end of a perturbation step is reset to zero.

If the input deck is stored in the file "problem.inp", where "problem" stands for any name, the eigenfrequencies are stored in the "problem.dat" file. Furthermore, if the parameter STORAGE is set to yes (STORAGE=YES) on the *FREQUENCY card the eigenfrequencies, eigenmodes and mass matrix are stored in binary form in a "problem.eig" file for further use (e.g. in a linear dynamic step).

All output of the eigenmodes is normalized by means of the mass matrix, i.e. the generalized mass is one. The eigenvalue of the generalized eigenvalue problem is actually the square of the eigenfrequency. The eigenvalue is guaranteed to be real (the stiffness and mass matrices are symmetric; the only exception to this is if contact friction is included, which can lead to complex eigenfrequencies), but it is positive only for positive definite stiffness matrices. Due to

preloading the stiffness matrix is not necessarily positive definite. This can lead to purely imaginary eigenfrequencies which physically mean that the structure buckles.

Apart from the eigenfrequencies the total effective mass and total effective modal mass for all rigid body modes are also calculated and stored in the .dat-file. There are six rigid body modes, three translations and three rotations. Let us call any of these $\{R\}$. It is a vector corresponding to a unit rigid body mode, e.g. a unit translation in the global x-direction. The participation factors P_i are calculated by

$$P_i = \{U_i\}^T [M]\{R\}. \tag{191}$$

They reflect the degree of participation of each mode in the selected rigid body motion. Recall that the modes are mass-normalized, consequently the unit of the mode is $1/\sqrt{\text{mass}}$, the unit of the rigid body motion is length. The effective modal mass is defined by P_i^2, the total effective modal mass by

$$\sum_i P_i^2 \tag{192}$$

(unit: mass $\cdot$length^2). The total effective mass is the size of the rigid motion, i.e. it is the internal product of the rigid motion with itself:

$$\{R\}^T [M]\{R\}. \tag{193}$$

If one would calculate infinitely many modes the total effective modal mass should be equal to the total effective mass. Since only a finite number of modes are calculated the total effective modal mass will be less. By comparing the total effective modal mass with the total effective mass one gains an impression whether enough modes were calculated to perform good modal dynamics calculation (at least for the rigid motions).

A special kind of frequency calculations is a cyclic symmetry calculation for which the keyword cards *SURFACE, *TIE, *CYCLIC SYMMETRY MODEL and *SELECT CYCLIC SYMMETRY MODES are available. This kind of calculation applies to structures consisting of identical sectors ordered in a cyclic way such as in Figure 119.

For such structures it is sufficient to model just one sector (also called datum sector) to obtain the eigenfrequencies and eigenmodes of the whole structure. The displacement values on the left and right boundary (or surfaces) of the datum sector are phase shifted. The shift depends on how many waves are looked for along the circumference of the structure. Figure 120 shows an eigenmode for a full disk exhibiting two complete waves along the circumference. This corresponds to four zero-crossings of the waves and a nodal diameter of two. This nodal diameter (also called cyclic symmetry mode number) can be considered as the number of waves, or also as the number of diameters in the structure along which the displacements are zero.

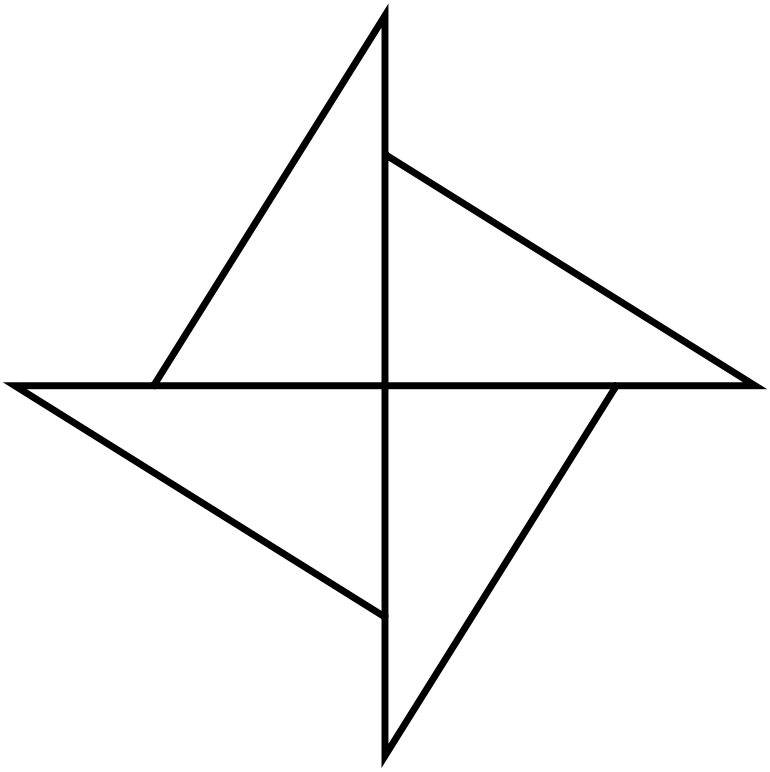


Figure 119: Cyclic symmetry structure consisting of four identical sectors

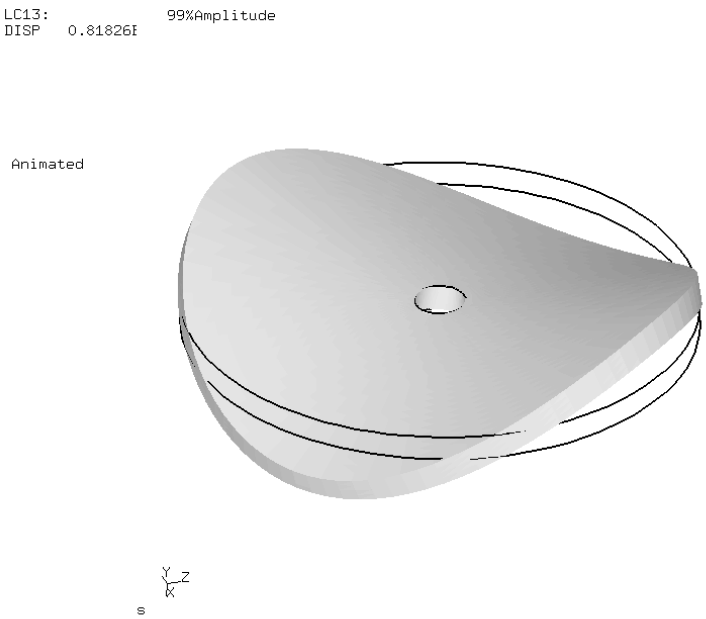


Figure 120: Eigenmode for a full disk with a nodal diameter of two

The lowest nodal diameter is zero and corresponds to a solution which is identical on the left and right boundary of the datum sector. For a structure consisting of N sectors, the highest feasible nodal diameter is N/2 for N even and (N-1)/2 for N odd. The nodal diameter is selected by the user on the *SELECT CYCLIC SYMMETRY MODES card. On the *CYCLIC SYMMETRY MODEL card, the number of base sectors fitting in 360° is to be provided. On the same card the user also indicates the number of sectors for which the solution is to be stored in the .frd file. In this way, the solution can be plotted for the whole structure, although the calculation was done for only one sector.

Mathematically the left and right boundary of the datum sector are coupled by MPC's with complex coefficients. This leads to a complex generalized eigenvalue problem with a Hermitian stiffness matrix, which can be reduced to a real eigenvalue problem the matrices of which are twice the size as those in the original problem.

The phase shift between left and right boundary of the datum sector is given by $2\pi N/M$, where N is the nodal diameter and M is the number of base sectors in 360°. Whereas N has to be an integer, CalculiX allows M to be a real number. In this way the user may enter a fictitious value for M, leading to arbitrary phase shifts between the left and right boundary of the datum sector (for advanced applications).

For models containing the axis of cyclic symmetry (e.g. a full disk), the

nodes on the symmetry axis are treated differently depending on whether the nodal diameter is 0, 1 or exceeds 1. For nodal diameter 0, these nodes are fixed in a plane perpendicular to the cyclic symmetry axis, for nodal diameter 1 they cannot move along the cyclic symmetry axis and for higher nodal diameters they cannot move at all. For these kind of structures calculations for nodal diameters 0 or 1 must be performed in separate steps.

Finally one word of caution on frequency calculations with axisymmetric elements. Right now, you will only get the eigenmodes corresponding to a nodal diameter of 0, i.e. all axisymmetric modes. If you would like to calculate asymmetric modes, please model a segment with volumetric elements and perform a cyclic symmetry analysis.

6.9.3 Complex frequency analysis

This procedure is used to calculate the eigenvalues and eigenmodes taking the Coriolis forces into account. The latter forces apply as soon as one performs calculations in a rotating frame of reference. Therefore, using the *DLOAD card to define a centrifugal speed in a *FREQUENCY step automatically triggers Coriolis forces. However, in a lot of applications the Coriolis forces are quite small and can be neglected. They may be important for very flexible rotating structures such as thin disks mounted on long rotating axes (rotor dynamics).

The presence of Coriolis forces changes the governing equation into

$$\left[M\right]\left\{\ddot{U}\right\} + \left[C\right]\left\{\dot{U}\right\} + \left[K\right]\left\{U\right\} = \left\{0\right\} \tag{194}$$

In a *FREQUENCY analysis the term with the Coriolis matrix $\left[C\right]$ is lacking. Now, the solution to the above equation is assumed to be a linear combination of the eigenmodes without Coriolis:

$$\left\{U(t)\right\} = \sum_i b_i \left\{U_i\right\} e^{i\omega t}. \tag{195}$$

Substituting this assumption into the governing equation and premultiplying the equation with $\left\{U_j\right\}^T$ leads to

$$\sum_i b_i \left\{U_j\right\}^T \left[C\right]\left\{U_i\right\} = \left[\frac{\omega_j^2 - \omega^2}{i\omega}\right] b_j. \tag{196}$$

Writing this equation for each value of j yields an eigenvalue problem of the form

$$\omega^2 \left\{b\right\} - i\omega \left[C^*\right]\left\{b\right\} - \left[Diag(\omega_j^2)\right]\left\{b\right\} = \left\{0\right\}. \tag{197}$$

This is a nonlinear eigenvalue problem which can be solved by a Newton-Raphson procedure. Starting values for the procedure are the eigenvalues of the *FREQUENCY step and some values in between. In rare cases an eigenvalue is missed (most often the last eigenvalue requested).

One can prove that the eigenvalues are real, the eigenmodes, however, are usually complex. Therefore, instead of requesting U underneath the *NODE FILE card yielding the real and imaginary part of the displacements it is rather instructive to request PU leading to the size and phase. With the latter information the mode can be properly visualized in CalculiX GraphiX.

Finally, notice that no *DLOAD card of type CORIO is needed in CalculiX. A loading of type CENTRIF in a preceding *STATIC step is sufficient. The usual procedure is indeed:

1. a *STATIC step to define the centrifugal force and calculate the deformation and stresses (may contain NLGEOM, but does not have to).

2. a *FREQUENCY step with PERTURBATION to calculate the eigenfrequencies and eigenmodes taking the centrifugal forces, stress stiffness and deformation stiffness into account. The *FREQUENCY card must include the parameter STORAGE=YES.

3. a *COMPLEX FREQUENCY,CORIOLIS step to include the Coriolis forces.

6.9.4 Buckling analysis

In a linear buckling analysis the initial stiffness matrix is augmented by the initial stress matrix corresponding to the load specified in the *BUCKLE step, multiplied with a factor. This so-called buckling factor is determined such that the resulting matrix has zero as its lowest eigenfrequency. Ultimately, the buckling load is the buckling factor multiplied with the step load. The buckling factor(s) are always stored in the .dat file. The load specified in a *BUCKLE step should not contain prescribed displacements.

If the perturbation parameter is not activated on the *STEP card, the initial stiffness matrix corresponds to the stiffness matrix of the unloaded structure.

If the perturbation parameter is activated, the initial stiffness matrix includes the deformation and stress stiffness matrix corresponding to the deformation and stress at the end of the last static or dynamic step performed previous to the buckling step, if any, and the material parameters are based on the temperature at the end of that step. In this way, the effect of previous loadings can be included in the buckling analysis.

In a buckling step, all loading previous to the step is removed and replaced by the buckling step's loading, which is reset to zero at the end of the buckling step. Thus, to continue a static step interrupted by a buckling step, the load has to be reapplied after the buckling step. Due to the intrinsic nonlinearity of temperature loading (the material properties usually change with temperature), this type of loading is not allowed in a linear buckling step. If temperature loading is an issue, a nonlinear static or dynamic calculation should be performed instead.

6.9.5 Modal dynamic analysis

In a modal dynamic analysis, triggered by the *MODAL DYNAMIC key word, the response of the structure to dynamic loading is assumed to be a linear combination of the lowest eigenmodes. These eigenmodes are recovered from a file "problem.eig", where "problem" stands for the name of the structure. These eigenmodes must have been determined in a previous step (STORAGE=YES on the *FREQUENCY card or on the *HEAT TRANSFER,FREQUENCY card), either in the same input deck, or in an input deck run previously. If, in the latter case, the eigenmode analysis exhibited cyclic symmetry (i.e. if the *SELECT CYCLIC SYMMETRY MODES card was used) make sure to use the CYCLIC SYMMETRY parameter on the *MODAL DYNAMIC card. The dynamic loading can be defined as a piecewise linear function by means of the *AMPLITUDE key word.

The displacement boundary conditions in a modal dynamic analysis should match zero boundary conditions in the same nodes and same directions in the step used for the determination of the eigenmodes. This corresponds to what is called base motion in ABAQUS. A typical application for nonzero boundary conditions is the base motion of a building due to an earthquake. Notice that in a modal dynamic analysis with base motion non-homogeneous multiple point constraints are not allowed. This applies in particular to single point constraints (boundary conditions) in a non-global coordinate system, such as a cylindrical coordinate system (defined by a *TRANSFORM card). Indeed, boundary conditions in a local coordinate system are internally transformed into non-homogeneous multiple point constraints. Consequently, in a modal dynamic analysis boundary conditions must be defined in the global Cartesian coordinate system.

Temperature loading or residual stresses are not allowed. If such loading arises, the direct integration dynamics procedure should be used.

Nonzero displacement boundary conditions in a modal dynamic analysis require the calculation of the first and second order time derivatives (velocity and acceleration) of the temporarily static solution induced by them. Indeed, based on the nonzero displacement boundary conditions (without any other loading) at time t a static solution can be determined for that time (that's why the stiffness matrix is included in the .eig file). If the nonzero displacement boundary conditions change with time, so will the induced static solution. Now, the solution to the dynamic problem is assumed to be the sum of this temporarily static solution and a linear combination of the lowest eigenmodes. To determine the first and second order time derivatives of the induced static solution, second order accurate finite difference schemes are used based on the solution at times $t - \Delta t$, t and $t + \Delta t$, where Δt is the time increment in the modal dynamic step. At the start of a modal dynamic analysis step the nonzero boundary conditions at the end of the previous step are assumed to have reached steady state (velocity and acceleration are zero).

Damping can be included by means of the *MODAL DAMPING key card. The damping models provided in CalculiX are direct damping and Rayleigh

damping. If direct damping is selected the viscous damping factor ζ can be defined for each mode separately. Rayleigh damping, assumes the damping matrix to be a linear combination of the problem's stiffness matrix and mass matrix. In both cases the problem is split according to its eigenmodes, and leads to ordinary differential equations. The results are exact for piecewise linear loading, apart from the inaccuracy due to the finite number of eigenmodes.

A modal dynamic analysis can also be performed for a cyclic symmetric structure. To this end, the eigenmodes must have been determined for all relevant modal diameters. For a cyclic modal dynamic analysis there are two limitations:

1. Nonzero boundary conditions are not allowed.

2. The displacements and velocities at the start of a step must be zero.

Special caution has to be applied if 1D and 2D elements are used. Since these elements are internally expanded into 3D elements, the application of boundary conditions and point forces to nodes requires the creation of multiple point constraints linking the original nodes to their expanded counterparts. These MPC's change the structure of the stiffness and mass matrix. However, the stiffness and mass matrix is stored in the .eig file in the *FREQUENCY step preceding the *MODAL DYNAMIC step. This is necessary, since the mass matrix is needed for the treatment of the initial conditions ([18]) and the stiffness matrix for taking nonzero boundary conditions into account. Summarizing, the *MODAL DYNAMIC step should not introduce point loads or nonzero boundary conditions in nodes in which no point force or boundary condition was defined in the *FREQUENCY step. The value of the point force and boundary conditions in the *FREQUENCY step can be set to zero. An example for the application of point forces to shells is given in shellf.inp of the test example set.

Special effort was undertaken to increase the computational speed for modal dynamic calculations. This is especially important if contact is used, since contact convergence can require very small time steps. If time is an issue for you, please take into account the following rules:

- Time varying loads slow down the execution.

- Loads applied in many elements slow down execution. Together with the previous rule this means that e.g. a constantly changing centrifugal load is very detrimental to the performance of the calculation.

- Nonzero displacements, centrifugal loads and gravity loads involve load changes in the complete mesh and slow down execution.

- Point loads act very local and are good for the performance.

- Use the parameter NSET on the *NODE FILE and *EL FILE card to limit output to a small set of nodes in order to accelerate the execution.

- Requesting element variables in the frd output slows down execution. So does requesting nodal forces, since these are derived from the stresses in the integration points. Limiting output to displacements (U) is very beneficial.

- Using the user subroutine cload.f (Section 8.4.2) slows down the execution, since this routine provides the user with the forces in the nodes at stake.

Summarizing, maximal speed will be obtained by applying a constant point load (Heaviside step function) in one node and requesting the displacements only in that node.

6.9.6 Steady state dynamics

In a steady state dynamics analysis, triggered by the *STEADY STATE DYNAMICS key word, the response of the structure to dynamic harmonic loading is assumed to be a linear combination of the lowest eigenmodes. This is very similar to the modal dynamics procedure, except that the load is harmonic in nature and that only the steady state response is of interest. The eigenmodes are recovered from a file "problem.eig", where "problem" stands for the name of the structure. These eigenmodes must have been determined in a previous step (STORAGE=YES on the *FREQUENCY card or on the *HEAT TRANSFER,FREQUENCY card), either in the same input deck, or in an input deck run previously. The dynamic harmonic loading is defined by its amplitude using the usual keyword cards such as *CLOAD and a frequency interval specified underneath the *STEADY STATE DYNAMICS card. The load amplitudes can be modified by means of a *AMPLITUDE key word, which is interpreted as load factor versus frequency (instead of versus time). The displacement boundary conditions in a modal dynamic analysis should match zero boundary conditions in the same nodes and same directions in the step used for the determination of the eigenmodes. Temperature loading or residual stresses are not allowed. If such loading arises, the direct integration dynamics procedure should be used.

One can define loading which is shifted by 90° by using the parameter LOAD CASE = 2 on the loading cards (e.g. *CLOAD).

The frequency range is specified by its lower and upper bound. The number of data points within this range n can also be defined by the user. If no eigenvalues occur within the specified range, this is the total number of data points taken, i.e. including the lower frequency bound and the upper frequency bound. If one or more eigenvalues fall within the specified range, $n-2$ points are taken in between the lower frequency bound and the lowest eigenfrequency in the range, $n-2$ between any subsequent eigenfrequencies in the range and $n-2$ points in between the highest eigenfrequency in the range and upper frequency bound. In addition, the eigenfrequencies are also included in the data points. Consequently, if m eigenfrequencies belong to the specified range, $(m+1)(n-2)+m+2 = nm-m+n$ data points are taken. They are equally spaced in between the fixed points (lower frequency bound, upper frequency

bound and eigenfrequencies) if the user specifies a bias equal to 1. If a different bias is specified, the data points are concentrated about the fixed points.

Damping can be included by means of the *MODAL DAMPING key card. The damping model provided in CalculiX is the Rayleigh damping, which assumes the damping matrix to be a linear combination of the problem's stiffness matrix and mass matrix. This splits the problem according to its eigenmodes, and leads to ordinary differential equations. The results are exact for piecewise linear loading, apart from the inaccuracy due to the finite number of eigenmodes. For nonharmonic loading, triggered by the parameter HARMONIC=NO on the *STEADY STATE DYNAMICS card, the loading across one period is not harmonic and has to be specified in the time domain. To this end the user can specify the starting time and the final time of one period and describe the loading within this period with *AMPLITUDE cards. Default is the interval $[0., 1.]$ and step loading. Notice that for nonharmonic loading the *AMPLITUDE cards describe amplitude versus TIME. Internally, the nonharmonic loading is expanded into a Fourier series. The user can specify the number of terms which should be used for this expansion, default is 20. The remaining input is the same as for harmonic loading, i.e. the user specifies a frequency range, the number of data points within this range and the bias. The comments above for harmonic loading also apply here, except that, since the loading is defined in the time domain, the LOAD CASE parameter does not make sense here, i.e. LOAD CASE = 1 by default.

A steady state dynamic analysis can also be performed for a cyclic symmetric structure. To this end, the eigenmodes must have been determined for all relevant modal diameters. For a cyclic steady state dynamic analysis there are three limitations:

1. Nonzero boundary conditions are not allowed.
2. The displacements and velocities at the start of a step must be zero.
3. Dashpot elements are not allowed.

The output of a steady state dynamics calculation is complex, i.e. it consists of a real and an imaginary part. Consequently, if the user saves the displacements to file, there will be two entries: first the real part of the displacement, then the imaginary part. This also applies to all other output variables such as temperature or stress. For the displacements, the temperatures and the stresses the user can request that these variables are stored as magnitude and phase (in that order) by selecting beneath the *NODE FILE card PU, PNT and PHS instead of U, NT and S respectively. This does not apply to the *NODE PRINT card.

Special caution has to be applied if 1D and 2D elements are used. Since these elements are internally expanded into 3D elements, the application of boundary conditions and point forces to nodes requires the creation of multiple point constraints linking the original nodes to their expanded counterparts. These MPC's change the structure of the stiffness and mass matrix. However,

the stiffness and mass matrix is stored in the .eig file in the *FREQUENCY step preceding the *STEADY STATE DYNAMICS step. This is necessary, since the mass matrix is needed for the treatment of the initial conditions ([18]) and the stiffness matrix for taking nonzero boundary conditions into account. Summarizing, the *STEADY STATE DYNAMICS step should not introduce point loads or nonzero boundary conditions in nodes in which no point force or boundary condition was defined in the *FREQUENCY step. The value of the point force and boundary conditions in the *FREQUENCY step can be set to zero. An example for the application of point forces to shells is given in shellf.inp of the test example set.

6.9.7 Direct integration dynamic analysis

In a direct integration dynamic analysis, activated by the *DYNAMIC key word, the equation of motion is integrated in time using the α-method developed by Hilber, Hughes and Taylor [53]. The parameter α lies in the interval [-1/3,0] and controls the high frequency dissipation: α=0 corresponds to the classical Newmark method inducing no dissipation at all, while α=-1/3 corresponds to maximum dissipation. The user can choose between an implicit and explicit version of the algorithm. The implicit version (default) is unconditionally stable.

In the explicit version, triggered by the parameter EXPLICIT in the *DYNAMIC keyword card, the mass matrix is lumped, and a forward integration scheme is used so that the solution can be calculated without solving a system of equations. Each iteration is much faster than with the implicit scheme. However, the explicit scheme is only conditionally stable: the maximum time step size is proportional to the time a mechanical wave needs to cross the smallest element in the mesh. For linear elements the proportionality factor is 1., for quadratic elements it is $1/\sqrt{6}$. For elastic materials, the wave speed in a rod is $\sqrt{E/\rho}$, where E is Young's modulus and ρ is the material density.

6.9.8 Heat transfer

In a heat transfer analysis, triggered by the *HEAT TRANSFER procedure card, the temperature is the independent degree of freedom. In essence, the energy equation is solved subject to temperature and flux boundary conditions ([18]). For steady-state calculations it leads to a Laplace-type equation.

The governing equation for heat transfer reads

$$\nabla \cdot (-\boldsymbol{\kappa} \cdot \nabla T) + \rho c \dot{T} = \rho h \tag{198}$$

where $\boldsymbol{\kappa}$ contains the conduction coefficients, ρ is the density, h the heat generation per unit of mass and c is the specific heat.

The temperature can be defined using the *BOUNDARY card using degree of freedom 11. Flux type boundary conditions can consist of any combination of the following:

1. Concentrated flux, applied to nodes, using the *CFLUX card (degree of freedom 11)

2. Distributed flux, applied to surfaces or volumes, using the *DFLUX card

3. Convective flux defined by a *FILM card. It satisfies the equation

$$q = h(T - T_0) \tag{199}$$

   where q is the a flux normal to the surface, h is the film coefficient, T is the body temperature and T_0 is the environment temperature (also called sink temperature). CalculiX can also be used for forced convection calculations, in which the sink temperature is an unknown too. This applied to all kinds of surfaces cooled by fluids or gases.

4. Radiative flux defined by a *RADIATE card. The equation reads

$$q = \epsilon(\theta^4 - \theta_0^4) \tag{200}$$

   where q is a flux normal to the surface, ϵ is the emissivity, θ is the absolute body temperature (Kelvin) and θ_0 is the absolute environment temperature (also called sink temperature). The emissivity takes values between 0 and 1. A zero value applied to a body with no absorption nor emission and 100 % reflection. A value of 1 applies to a black body. The radiation is assumed to be diffuse (independent of the direction of emission) and gray (independent of the emitted wave length). CalculiX can also be used for cavity radiation, simulating the radiation interaction of several surfaces. In that case, the viewfactors are calculated, see also [34] for the fundamentals of heat transfer and [6] for the calculation of viewfactors.

   The calculation of viewfactors involves the solution of a four-fold integral. By using analytical formulas derived by Lambert this integral can be reduced to a two-fold integral. This is applied in CalculiX right now: the interacting surfaces are triangulated and the viewfactor between two triangles is calculated by taking a one-point integration for the base triangle (in the center of gravity) and the analytical formula for the integration over the other triangles covering a hemisphere about the base triangle. One can switch to a more accurate integration over the base triangle by increasing the variable "factor" in subroutine radmatrix, look at the comments in that subroutine. This, however, will increase the computational time.

For a heat transfer analysis the conductivity coefficients of the material are needed (using the *CONDUCTIVITY card) and for transient calculations the heat capacity (using the *SPECIFIC HEAT card). Furthermore, for radiation boundary conditions the *PHYSICAL CONSTANTS card is needed, specifying absolute zero in the user's temperature scale and the Boltzmann constant.

Table 9: Correspondence between the heat equation and the gas momentum equation.

heat quantity	gas quantity
T	p
$\boldsymbol{q}$	$\rho_0(\boldsymbol{a}-\boldsymbol{f})$
q_n	$\rho_0(a_n-f_n)$
$\boldsymbol{\kappa}$	$\boldsymbol{I}$
ρh	$-\rho_0\nabla\cdot\boldsymbol{f}$
ρc	$\frac{1}{c_0^2}$

Notice that a phase transition can be modeled by a local sharp maximum of the specific heat. The energy U per unit of mass needed to complete the phase transition satisfies

$$U=\int_{T_0}^{T_1} C dT, \tag{201}$$

where C is the specific heat and $[T_0,T_1]$ is the temperature interval within which the phase transition takes place.

6.9.9 Acoustics

Linear acoustic calculations in gas are very similar to heat transfer calculations. Indeed, the pressure variation in a space with uniform basis pressure p_0 and density ρ_0 (and consequently uniform temperature T_0 due to the gas law) satisfies

$$\nabla\cdot(-\boldsymbol{I}\cdot\nabla p)+\frac{1}{c_0^2}\ddot{p}=-\rho_0\nabla\cdot\boldsymbol{f}, \tag{202}$$

where $\boldsymbol{I}$ is the second order unit tensor (or, for simplicity, unit matrix) and c_0 is the speed of sound satisfying:

$$c_0=\sqrt{\gamma R T_0}. \tag{203}$$

γ is the ratio of the heat capacity at constant pressure divided by the heat capacity at constant volume ($\gamma=1.4$ for normal air), R is the specific gas constant ($R=287J/(kgK)$ for normal air) and T_0 is the absolute basis temperature (in K). Furthermore, the balance of momentum reduces to:

$$\nabla p=\rho_0(\boldsymbol{f}-\boldsymbol{a}). \tag{204}$$

For details, the reader is referred to [20] and [2]. Equation (202) is the well-known wave equation. By comparison with the heat equation, the correspondence in Table (9) arises.

Notice, however, that the time derivative in the heat equation is first order, in the gas momentum equation it is second order. This means that the transient heat transfer capability in CalculiX can NOT be used for the gas equation. However, the frequency option can be used and the resulting eigenmodes can be taken for a subsequent modal dynamic or steady state dynamics analysis. Recall that the governing equation for solids also has a second order time derivative ([18]).

For the driving terms one obtains:

$$\int_A \rho_0(a_n - f_n)dA - \int_V \rho_0 \nabla \cdot \boldsymbol{f} dV = \int_A \rho_0 a_n dA, \tag{205}$$

which means that the equivalent of the normal heat flux at the boundary is the basis density multiplied with the acceleration. Consequently, at the boundary either the pressure must be known or the acceleration.

6.9.10 Shallow water motion

For incompressible fluids integration of the governing equations over the fluid depth and subsequent linearization leads to the following equation:

$$\nabla \cdot (-gH\boldsymbol{I} \cdot \nabla\eta) + \ddot{\eta} = 0, \tag{206}$$

where g is the earth acceleration, H is the fluid depth measured from a reference level, $\boldsymbol{I}$ is the unit tensor and η is the fluid height with respect to the reference level. Usually the fluid level at rest is taken as reference level. The derivation of the equation is described in [78]. The following assumptions are made:

- no viscosity
- no Coriolis forces
- no convective acceleration
- $H + \eta \approx H$

Due to the integration process the above equation is two-dimensional, i.e. only the surface of the fluid has to be meshed. By comparison with the heat equation, the correspondence in Table (10) arises. Therefore, shallow water motion can be simulated using the *HEAT TRANSFER procedure.

The quantity $\overline{\boldsymbol{v}}$ is the average velocity over the depth and $\overline{v}_n$ is its component orthogonal to the boundary of the domain. Due to the averaging the equations hold for small depths only (shallow water approximation). Notice that the equivalence of the heat conduction coefficient is proportional to the depth, which is a geometric quantity. For a different depth a different conduction coefficient must be defined.

There is no real two-dimensional element in CalculiX. Therefore, the two-dimensional Helmholtz equation has to be simulated by expanding the two-dimensional fluid surface to a three-dimensional layer with constant width and

Table 10: Correspondence between the heat equation and the shallow water equation.

heat quantity	shallow water quantity
T	η
$\boldsymbol{q}$	$\frac{\partial}{\partial t}(H\overline{\boldsymbol{v}})$
q_n	$H\frac{\partial}{\partial t}(\overline{v}_n)$
$\boldsymbol{\kappa}$	$Hg\boldsymbol{I}$
ρh	–
ρc	1

applying the boundary conditions in such a way that no variation occurs over the width.

Notice that, similar to the acoustic equations, the shallow water equations are of the Helmholtz type leading to a hyperbolic system. For instationary applications eigenmodes can be calculated and a modal analysis performed.

6.9.11 Hydrodynamic lubrication

In hydrodynamic lubrication a thin oil film constitutes the interface between a static part and a part rotating at high speed in all kinds of bearings. A quantity of major interest to engineers is the load bearing capacity of the film, expressed by the pressure. Integrating the hydrodynamic equations over the width of the thin film leads to the following equation [26]:

$$\nabla \cdot (-\frac{h^3\overline{\rho}}{12\mu_v}\boldsymbol{I} \cdot \nabla p) = -\left(\frac{\boldsymbol{v}_b + \boldsymbol{v}_a}{2}\right) \cdot \nabla(h\overline{\rho}) - \frac{\partial(h\overline{\rho})}{\partial t} - \dot{m}_\Omega, \tag{207}$$

where h is the film thickness, $\overline{\rho}$ is the mean density across the thickness, p is the pressure, μ_v is the dynamic viscosity of the fluid, $\boldsymbol{v}_a$ is the velocity on one side of the film, $\boldsymbol{v}_b$ is the velocity at the other side of the film and $\dot{m}_\Omega$ is the resulting volumetric flux (volume per second and per unit of area) leaving the film through the porous walls (positive if leaving the fluid). This term is zero if the walls are not porous.

For practical calculations the density and thickness of the film is assumed to be known, the pressure is the unknown. By comparison with the heat equation, the correspondence in Table (11) arises. $\overline{\boldsymbol{v}}$ is the mean velocity over the film, $\overline{v}_n$ its component orthogonal to the boundary. Since the governing equation is the result of an integration across the film thickness, it is again two-dimensional and applies in the present form to a plane film. Furthermore, observe that it is a steady state equation (the time change of the density on the right hand side is assumed known) and as such it is a Poisson equation. Here too, just like for the shallow water equation, the heat transfer equivalent of a spatially varying layer thickness is a spatially varying conductivity coefficient.

Table 11: Correspondence between the heat equation and the dynamic lubrication equation.

heat quantity	dynamic lubrication quantity
T	p
$\boldsymbol{q}$	$\overline{\rho}h\overline{\boldsymbol{v}}$
q_n	$\overline{\rho}h\overline{v}_n$
$\boldsymbol{\kappa}$	$\frac{h^3\overline{\rho}}{12\mu_v}\boldsymbol{I}$
ρh	$-\left(\frac{\boldsymbol{v}_b+\boldsymbol{v}_a}{2}\right)\cdot\nabla(h\overline{\rho})-\frac{\partial(h\overline{\rho})}{\partial t}-\dot{m}_\Omega$
ρc	$-$

Table 12: Correspondence between the heat equation and the equation for incompressible irrotational inviscid flow.

heat quantity	irrotational flow quantity
T	ϕ
$\boldsymbol{q}$	$\boldsymbol{v}$
q_n	v_n
$\boldsymbol{\kappa}$	$\boldsymbol{I}$
ρh	0
ρc	$-$

6.9.12 Irrotational incompressible inviscid flow

If incompressible flow is irrotational a potential ϕ exists for the velocity field such that $\boldsymbol{v}=-\nabla\phi$. Furthermore, if the flow is inviscid one can prove that if a flow is irrotational at any instant in time, it remains irrotational for all subsequent time instants [78]. The continuity equation now reads

$$\nabla\cdot(-\boldsymbol{I}\cdot\nabla\phi)=0, \tag{208}$$

and the balance of momentum for gravitational flow yields

$$\frac{\partial\boldsymbol{v}}{\partial t}+\nabla\left(\frac{p}{\rho_0}+\frac{\boldsymbol{v}\cdot\boldsymbol{v}}{2}+gz\right)=0, \tag{209}$$

where g is the earth acceleration, p is the pressure, ρ_0 is the density and z is the coordinate in earth direction. By comparison with the heat equation, the correspondence in Table (12) arises.

Once ϕ is determined, the velocity $\boldsymbol{v}$ is obtained by differentiation and the pressure p can be calculated through the balance of momentum. Although irrotational incompressible inviscid flow sounds very special, the application field is rather large. Flow starting from rest is irrotational since the initial field is irrotational. Flow at speeds below 0.3 times the speed of sound can be

considered to be incompressible. Finally, the flow outside the tiny boundary layer around an object is inviscid. A favorite examples is the flow around a wing profile. However, if the boundary layer separates and vortices arise the above theory cannot be used any more. For further applications see [37].

6.9.13 Electrostatics

The governing equations of electrostatics are

$$\boldsymbol{E} = -\nabla V \tag{210}$$

and

$$\nabla \cdot \boldsymbol{E} = \frac{\rho^e}{\epsilon_0}, \tag{211}$$

where $\boldsymbol{E}$ is the electric field, V is the electric potential, ρ^e is the electric charge density and ϵ_0 is the permittivity of free space ($\epsilon_0 = 8.8542 \times 10^{-12}$ C^2/Nm^2). The electric field $\boldsymbol{E}$ is the force on a unit charge.

In metals, it is linked to the current density $\boldsymbol{j}$ by the electric conductivity σ_c [5]:

$$\boldsymbol{j} = \sigma_c \boldsymbol{E}. \tag{212}$$

In free space, the electric field is locally orthogonal to a conducting surface. Near the surface the size of the electric field is proportional to the surface charge density σ[22]:

$$\sigma = E_n \epsilon_0. \tag{213}$$

Substituting Equation (210) into Equation (211) yields the governing equation

$$\nabla \cdot (-\boldsymbol{I} \cdot \nabla V) = \frac{\rho^e}{\epsilon_0}. \tag{214}$$

Accordingly, by comparison with the heat equation, the correspondence in Table (13) arises. Notice that the electrostatics equation is a steady state equation, and there is no equivalent to the heat capacity term.

An application of electrostatics is the potential drop technique for crack propagation measurements: a predefined current is sent through a conducting specimen. Due to crack propagation the specimen section is reduced and its electric resistance increases. This leads to an increase of the electric potential across the specimen. A finite element calculation for the specimen (electrostatic equation with $\rho^e = 0$) can determine the relationship between the potential and the crack length. This calibration curve can be used to derive the actual crack length from potential measurements during the test.

Another application is the calculation of the capacitance of a capacitor. Assuming the space within the capacitor to be filled with air, the electrostatic

Table 13: Correspondence between the heat equation and the equation for electrostatics (metals and free space).

heat	electrostatics
T	V
$\boldsymbol{q}$	$\boldsymbol{E}$
q_n	$E_n = \frac{j_n}{\sigma}$
$\boldsymbol{\kappa}$	$\boldsymbol{I}$
ρh	$\frac{\rho^e}{\epsilon_0}$
ρc	$-$

equation with $\rho^e = 0$ applies (since there is no charge within the capacitor). Fixing the electric potential on each side of the capacitor (to e.g. zero and one), the electric field can be calculated by the thermal analogy. This field leads to a surface charge density by Equation (213). Integrating this surface charge leads to the total charge. The capacitance is defined as this total charge divided by the electric potential difference (one in our equation).

For dielectric applications Equation (211) is modified into

$$\nabla \cdot \boldsymbol{D} = \rho^f, \tag{215}$$

where $\boldsymbol{D}$ is the electric displacement and ρ^f is the free charge density [22]. The electric displacement is coupled with the electric field by

$$\boldsymbol{D} = \epsilon \boldsymbol{E} = \epsilon_0 \epsilon_r \boldsymbol{E}, \tag{216}$$

where ϵ is the permittivity and ϵ_r is the relative permittivity (usually $\epsilon_r > 1$, e.g. for silicon ϵ_r=11.68). Now, the governing equation yields

$$\nabla \cdot (-\epsilon \boldsymbol{I} \cdot \nabla V) = \rho^f \tag{217}$$

and the analogy in Table (14) arises. The equivalent of Equation (213) now reads

$$\sigma = D_n. \tag{218}$$

The thermal equivalent of the total charge on a conductor is the total heat flow. Notice that ϵ may be a second-order tensor for anisotropic materials.

6.9.14 Stationary groundwater flow

The governing equations of stationary groundwater flow are [27]

$$\boldsymbol{v} = -\boldsymbol{k} \cdot \nabla h \tag{219}$$

Table 14: Correspondence between the heat equation and the equation for electrostatics (dielectric media).

heat	electrostatics
T	V
$\boldsymbol{q}$	$\boldsymbol{D}$
q_n	D_n
$\boldsymbol{\kappa}$	$\epsilon \boldsymbol{I}$
ρh	ρ^f
ρc	$-$

Table 15: Correspondence between the heat equation and the equation for groundwater flow.

heat	groundwater flow
T	h
$\boldsymbol{q}$	$\boldsymbol{v}$
q_n	v_n
$\boldsymbol{\kappa}$	$\boldsymbol{k}$
ρh	0
ρc	$-$

(also called Darcy's law) and

$$\nabla \cdot \boldsymbol{v} = 0, \tag{220}$$

where $\boldsymbol{v}$ is the discharge velocity, $\boldsymbol{k}$ is the permeability tensor and h is the total head defined by

$$h = \frac{p}{\rho g} + z. \tag{221}$$

In the latter equation p is the groundwater pressure, ρ is its density and z is the height with respect to a reference level. The discharge velocity is the quantity of fluid that flows through a unit of total area of the porous medium in a unit of time.

The resulting equation now reads

$$\nabla \cdot (-\boldsymbol{k} \cdot \nabla h) = 0. \tag{222}$$

Accordingly, by comparison with the heat equation, the correspondence in Table (15) arises. Notice that the groundwater flow equation is a steady state equation, and there is no equivalent to the heat capacity term.

Possible boundary conditions are:

1. unpermeable surface under water. Taking the water surface as reference height and denoting the air pressure by p_0 one obtains for the total head:

$$h = \frac{p_0 - \rho g z}{\rho g} + z = \frac{p_0}{\rho g}. \tag{223}$$

2. surface of seepage, i.e. the interface between ground and air. One obtains:

$$h = \frac{p_0}{\rho g} + z. \tag{224}$$

3. unpermeable boundary: $v_n = 0$

4. free surface, i.e. the upper boundary of the groundwater flow within the ground. Here, two conditions must be satisfied: along the free surface one has

$$h = \frac{p_0}{\rho g} + z. \tag{225}$$

In the direction $\boldsymbol{n}$ perpendicular to the free surface $v_n = 0$ must be satisfied. However, the problem is that the exact location of the free surface is not known. It has to be determined iteratively until both equations are satisfied.

6.9.15 Diffusion mass transfer in a stationary medium

The governing equations for diffusion mass transfer are [34]

$$\boldsymbol{j}_A = -\rho \boldsymbol{D}_{AB} \nabla m_A \tag{226}$$

and

$$\nabla \cdot \boldsymbol{j}_A + \dot{n_A} = \frac{\partial \rho_A}{\partial t}, \tag{227}$$

where

$$m_A = \frac{\rho_A}{\rho_A + \rho_B} \tag{228}$$

and

$$\rho = \rho_A + \rho_B. \tag{229}$$

In these equations $\boldsymbol{j}_A$ is the mass flux of species A, $\boldsymbol{D}_{AB}$ is the mass diffusivity, m_A is the mass fraction of species A and ρ_A is the density of species A. Furthermore, $\dot{n_A}$ is the rate of increase of the mass of species A per unit volume of the mixture. Another way of formulating this is:

$$\boldsymbol{J}_A^* = -C \boldsymbol{D}_{AB} \nabla x_A \tag{230}$$

Table 16: Correspondence between the heat equation and mass diffusion equation.

heat	mass diffusion	
T	ρ	C_A
$\boldsymbol{q}$	$\boldsymbol{j}_A$	$\boldsymbol{J}_A^*$
q_n	j_{An}	J_{A^*n}
$\boldsymbol{\kappa}$	$\boldsymbol{D}_{AB}$	$\boldsymbol{D}_{AB}$
ρh	$\dot{n_A}$	$\dot{N}_A$
ρc	1	1

and

$$\nabla \cdot \boldsymbol{J}_A^* + \dot{N}_A = \frac{\partial C_A}{\partial t}. \tag{231}$$

where

$$x_A = \frac{C_A}{C_A + C_B} \tag{232}$$

and

$$C = C_A + C_B. \tag{233}$$

Here, $\boldsymbol{J}_A^*$ is the molar flux of species A, $\boldsymbol{D}_{AB}$ is the mass diffusivity, x_A is the mole fraction of species A and C_A is the molar concentration of species A. Furthermore, $\dot{N}_A$ is the rate of increase of the molar concentration of species A.

The resulting equation now reads

$$\nabla \cdot (-\rho \boldsymbol{D}_{AB} \cdot \nabla m_A) + \frac{\partial \rho_A}{\partial t} = \dot{n_A}. \tag{234}$$

or

$$\nabla \cdot (-C \boldsymbol{D}_{AB} \cdot \nabla x_A) + \frac{\partial C_A}{\partial t} = \dot{N}_A. \tag{235}$$

If C and ρ are constant, these equations reduce to:

$$\nabla \cdot (-\boldsymbol{D}_{AB} \cdot \nabla \rho_A) + \frac{\partial \rho_A}{\partial t} = \dot{n_A}. \tag{236}$$

or

$$\nabla \cdot (-\boldsymbol{D}_{AB} \cdot \nabla C_A) + \frac{\partial C_A}{\partial t} = \dot{N}_A. \tag{237}$$

Accordingly, by comparison with the heat equation, the correspondence in Table (16) arises.

6.9.16 Aerodynamic Networks

Aerodynamic networks are made of a concatenation of network elements filled with a compressible medium which can be considered as an ideal gas. An ideal gas satisfies

$$p = \rho R \theta, \tag{238}$$

where p is the pressure, ρ is the density, R is the specific gas constant and θ is the absolute temperature. A network element (see section 6.2.27) consists of three nodes: in the corner nodes the temperature and pressure are the unknowns, in the midside node the mass flow is unknown. The corner nodes play the role of crossing points in the network, whereas the midside nodes represent the flow within one element. To determine these unknowns, three types of equations are available: conservation of mass and conservation of energy in the corner nodes and conservation of momentum in the midside node. Right now, only stationary flow is considered.

The stationary form of the conservation of mass for compressible fluids is expressed by:

$$\nabla \cdot (\rho \mathbf{v}) = 0 \tag{239}$$

where $\mathbf{v}$ the velocity vector. Integration over all elements connected to corner node i yields:

$$\sum_{j \in \text{in}} \dot{m}_{ij} = \sum_{j \in \text{out}} \dot{m}_{ij}, \tag{240}$$

where $\dot{m}_{ij}$ is the mass flow from node i to node j or vice versa. In the above equation $\dot{m}_{ij}$ is always positive.

The conservation of momentum or element equations are specific for each type of fluid section attributed to the element and are discussed in Section 6.4 on fluid sections. For an element with corner nodes i,j it is generally of the form $f(p_{toti}, \theta_{toti}, \dot{m}_{ij}, p_{totj}) = 0$ (for positive $\dot{m}_{ij}$, where p is the total pressure and θ_{tot} is the total temperature), although more complex relationships exist. Notice in particular that the temperature pops up in this equation (this is not the case for hydraulic networks).

The conservation of energy in stationary form requires ([25]):

$$\nabla \cdot (\rho h_{tot} \mathbf{v}) = -\nabla \cdot \mathbf{q} + \rho h^{\theta} + \rho \mathbf{f} \cdot \mathbf{v}, \tag{241}$$

where $\mathbf{q}$ is the external heat flux, h^{θ} is the body flux per unit of mass and $\mathbf{f}$ is the body force per unit of mass. h_{tot} is the total enthalpy satisfying:

$$h_{tot} = c_p \theta + \frac{\mathbf{v} \cdot \mathbf{v}}{2}, \tag{242}$$

where c_p is the specific heat at constant pressure and θ is the absolute temperature (in Kelvin). This latter formula only applies if c_p is considered to be independent of the temperature. This is largely true for a lot of industrial

applications. In this connection the reader be reminded of the definition of total temperature and total pressure (also called stagnation temperature and stagnation pressure, respectively):

$$\theta_{tot} = \theta + \frac{\mathbf{v} \cdot \mathbf{v}}{2c_p}, \tag{243}$$

and

$$\frac{p_{tot}}{p} = \left(\frac{\theta_{tot}}{\theta}\right)^{\frac{\kappa}{\kappa-1}}, \tag{244}$$

where $\kappa = c_p/c_v$. θ and p are also called the static temperature and static pressure, respectively.

If the corner nodes of the elements are considered to be large chambers, the velocity $\mathbf{v}$ is zero. In that case, the total quantities reduce to the static ones, and integration of the energy equation over all elements belonging to end node i yields [18]:

$$c_p(\theta_i) \sum_{j \in \text{in}} \theta_j \dot{m}_{ij} - c_p(\theta_i)\theta_i \sum_{j \in \text{out}} \dot{m}_{ij} + \overline{h}(\theta_i, \theta)(\theta - \theta_i) + m_i h_i^{\theta} = 0, \tag{245}$$

where $\overline{h}(\theta_i, \theta)$ is the convection coefficient with the walls. Notice that, although this is not really correct, a slight temperature dependence of c_p is provided for. If one assumes that all flow entering a node must also leave it and taking for both the c_p value corresponding to the mean temperature value of the entering flow, one arrives at:

$$\sum_{j \in \text{in}} c_p(\theta_m)(\theta_j - \theta_i)\dot{m}_{ij} + \overline{h}(\theta_i, \theta)(\theta - \theta_i) + m_i h_i^{\theta} = 0. \tag{246}$$

where $\theta_m = (\theta_i + \theta_j)/2$.

The calculation of aerodynamic networks is triggered by the *HEAT TRANSFER keyword card. Indeed, such a network frequently produces convective boundary conditions for solid mechanics heat transfer calculations. However, network calculations can also be performed on their own.

A particularly delicate issue in networks is the number of boundary conditions which is necessary to get a unique solution. To avoid ending up with more or less equations than unknowns, the following rules should be obeyed:

- The pressure and temperature should be known in those nodes where mass flow is entering the network. Since it is not always clear whether at a specific location mass flow is entering or leaving, it is advisable (though not necessary) to prescribe the pressure and temperature at all external connections, i.e in the nodes connected to dummy network elements.
- A node where the pressure is prescribed should be connected to a dummy network element. For instance, if you have a closed circuit add an extra dummy network element to the node in which you prescribe the pressure.

Output variables are the mass flow (key MF on the *NODE PRINT or *NODE FILE card), the total pressure (key PN — network pressure — on the *NODE PRINT card and PT on the *NODE FILE card) and the total temperature (key NT on the *NODE PRINT card and TT on the *NODE FILE card). Notice that the labels for the *NODE PRINT keyword are more generic in nature, for the *NODE FILE keyword they are more specific. These are the primary variables in the network. In addition, the user can also request the static temperature (key TS on the *NODE FILE card). Internally, in network nodes, components one to three of the structural displacement field are used for the mass flow, the total pressure and the static temperature, respectively. So their output can also be obtained by requesting U on the *NODE PRINT card.

6.9.17 Hydraulic Networks

Hydraulic networks are made of a concatenation of network elements (see section 6.2.27) filled with an incompressible medium. A network element consists of three nodes: in the corner nodes the temperature and pressure are the unknowns, in the midside node the mass flow is unknown. The corner nodes play the role of crossing points in the network, whereas the midside nodes represent the flow within one element. To determine these unknowns, three types of equations are available: conservation of mass and conservation of energy in the corner nodes and conservation of momentum in the midside node. Right now, only stationary flow is considered.

The stationary form of the conservation of mass for incompressible fluids is expressed by:

$$\nabla \cdot \mathbf{v} = 0 \tag{247}$$

where ρ is the density and $\mathbf{v}$ the velocity vector. Integration over all elements connected to an corner node yields:

$$\sum_{j \in \text{in}} \dot{m}_{ij} = \sum_{j \in \text{out}} \dot{m}_{ij}, \tag{248}$$

where $\dot{m}_{ij}$ is the mass flow from node i to node j or vice versa. In the above equation $\dot{m}_{ij}$ is always positive.

The conservation of momentum reduces to the Bernoulli equation. It is obtained by projecting the general momentum equation on a flow line within an element with corner nodes i and j and reads:

$$z_i + \frac{p_i}{\rho g} + \frac{\dot{m}_{ij}^2}{2\rho^2 A_i^2 g} = z_j + \frac{p_j}{\rho g} + \frac{\dot{m}_{ij}^2}{2\rho^2 A_j^2 g} + \Delta F_i^j. \tag{249}$$

Here, z is the height of the node, p the pressure, ρ the density, g the gravity acceleration, A the cross section in the node and ΔF_i^j is the head loss across the element. The head loss is positive if the flow runs from i to j, else it is negative (or has to be written on the other side of the equation). The head losses for different types of fluid sections are described in Section 6.5.

Notice that the height of the node is important, therefore, for hydraulic networks the gravity vector must be defined for each element using a *DLOAD card.

The conservation of energy in stationary form requires ([18]):

$$c_p \nabla \cdot (\rho \theta \mathbf{v}) = -\nabla \cdot \mathbf{q} + \rho h^\theta, \tag{250}$$

where $\mathbf{q}$ is the external heat flux, h^θ is the body flux per unit of mass, c_p is the specific heat at constant pressure (which, for a fluid, is also the specific heat at constant specific volume, i.e. $c_p = c_v$ [25]) and θ is the absolute temperature (in Kelvin). Integration of the energy equation over all elements belonging to end node i yields:

$$c_p(\theta_i) \sum_{j \in \text{in}} \theta_j \dot{m}_{ij} - c_p(\theta_i)\theta_i \sum_{j \in \text{out}} \dot{m}_{ij} + \overline{h}(\theta_i, \theta)(\theta - \theta_i) + m_i h_i^\theta = 0, \tag{251}$$

where $\overline{h}(\theta_i, \theta)$ is the convection coefficient with the walls. If one assumes that all flow entering a node must also leave it and taking for both the c_p value corresponding to the mean temperature value of the entering flow, one arrives at:

$$\sum_{j \in \text{in}} c_p(\theta_m)(\theta_j - \theta_i)\dot{m}_{ij} + \overline{h}(\theta_i, \theta)(\theta - \theta_i) + m_i h_i^\theta = 0. \tag{252}$$

where $\theta_m = (\theta_i + \theta_j)/2$.

The calculation of hydraulic networks is triggered by the *HEAT TRANSFER keyword card. Indeed, such a network frequently produces convective boundary conditions for solid mechanics heat transfer calculations. However, network calculations can also be performed on their own, i.e. it is allowed to do *HEAT TRANSFER calculations without any solid elements.

To determine appropriate boundary conditions for a hydraulic network the same rules apply as for aerodynamic networks.

Output variables are the mass flow (key MF on the *NODE PRINT or *NODE FILE card), the static pressure (key PN — network pressure — on the *NODE PRINT card and PS on the *NODE FILE card) and the total temperature (key NT on the *NODE PRINT card and TT on the *NODE FILE card). Notice that the labels for the *NODE PRINT keyword are more generic in nature, for the *NODE FILE keyword they are more specific. These are the primary variables in the network. Internally, in network nodes, components one to two of the structural displacement field are used for the mass flow and the static pressure, respectively. So their output can also be obtained by requesting U on the *NODE PRINT or *NODE FILE card.

Notice that for liquids the total temperature virtually coincides with the static temperature. Indeed, since

$$\theta_{tot} - \theta = v^2/(2c_p), \tag{253}$$

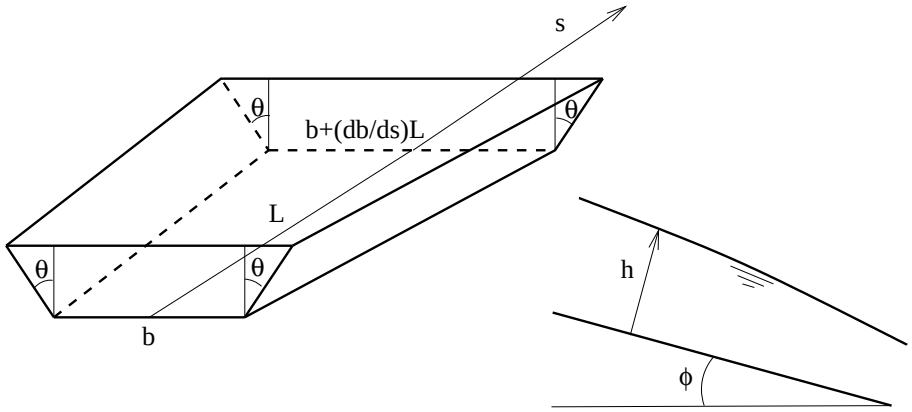


Figure 121: Channel geometry

the difference between total and static temperature for a fluid velocity of 5 m/s and $c_p = 4218$ J/(kg.K) (water) amounts to 0.0030 K. This is different from the gases since typical gas velocities are much higher (speed of sound is 340 m/s) and c_p for gases is usually lower.

6.9.18 Turbulent Flow in Open Channels

The turbulent flow in open channels can be approximated by one-dimensional network calculations. For the theoretical background the reader is referred to [16] and expecially [11] (in Dutch). The governing equation is the Bresse equation, which is a special form of the Bernoulli equation:

$$\frac{dh}{ds} = \frac{S_0 - S_f + \frac{1}{g}\frac{Q^2}{A^3}\frac{\partial A}{\partial s}}{\sqrt{1 - S_0^2 - \frac{Q^2 B}{gA^3}}}, \tag{254}$$

where (Figure 121) h is the water depth (measured perpendicular to the channel floor), s is the length along the bottom, $S_0 = \sin(\phi)$, where ϕ is the angle the channel floor makes with a horizontal line, S_f is a friction term, g is the earth acceleration, Q is the volumetric flow (mass flow divided by the fluid density), A is the area of the cross section $\frac{\partial A}{\partial s}$ is the change of the cross section with s keeping h fixed and B is the width of the channel at the fluid surface. The assumptions used to derive the Bresse equation are:

1. steady-state flow
2. each cross section is hydrostatic
3. the velocity is constant across each cross section
4. the velocity vector is perpendicular to each cross section.

For S_f several formulas have been proposed. In CalculiX the White-Colebrook and the Manning formula are implemented. The White-Colebrook formula reads

$$S_f = \frac{f}{8g}\frac{Q^2 P}{A^3}, \tag{255}$$

where f is the friction coefficient determined by Equation 27, and P is the wetted circumference of the cross section. The Manning form reads

$$S_f = \frac{n^2 Q^2 P^{4/3}}{A^{10/3}} \tag{256}$$

where n is the Manning coefficient, which has to be determined experimentally.

In CalculiX the channel cross section has to be trapezoidal (Figure 121). For this geometry the following relations apply:

$$A = h(b + h\tan\theta), \tag{257}$$

$$P = b + \frac{2h}{\cos\theta} \tag{258}$$

and

$$B = b + 2h\tan\theta. \tag{259}$$

Within an element the floor width b is allowed to change in a linear way. All other geometry parameters are invariable. Consequently:

$$\frac{\partial A}{\partial s} = h\frac{\partial b}{\partial s}. \tag{260}$$

The elements used in CalculiX for one-dimensional channel networks are regular network elements, in which the unknowns are the fluid depth and the temperature at the end nodes and the mass flow in the middle nodes. The equations at our disposal are the Bresse equation in the middle nodes (conservation of momentum), and the mass and energy conservation (Equations 248 and 252, respectively) at the end nodes.

Channel flow can be supercritical or subcritical. For supercritical flow the velocity exceeds the propagation speed c of a wave, which satisfies $c = \sqrt{gh}$. Defining the Froude number by $Fr = U/c$, where U is the velocity of the fluid, supercritical flow corresponds to $Fr > 1$. Supercritical flow is controlled by upstream boundary conditions. If the flow is subcritical ($Fr < 1$) it is controlled by downstream boundary conditions. In a subcritical flow disturbances propagate upstream and downstream, in a supercritical flow they propagation downstream only. A transition from supercritical to subcritical flow is called a hydraulic jump, a transition from subcritical to supercritical flow is a fall. At a jump the following equation is satisfied [16] (conservation of momentum):

$$A_2\dot{m}^2 + \rho^2 g\sqrt{1 - S_0^2}A_1^2 A_2 y_{G1} = A_1\dot{m}^2 + \rho^2 g\sqrt{1 - S_0^2}A_2^2 A_1 y_{G2}, \tag{261}$$

where A_1, A_2 are the cross sections before and after the jump, y_{G1} and y_{G2} are the centers of gravity of these sections, ρ is the fluid density and $\dot{m}$ is the mass flow. A fall can only occur at discontinuities in the channel geometry, e.g. at a discontinuous increase of the channel floor slope S_0. Available boundary conditions are the sluice gate, the weir and the infinite reservoir. They are described in Section 6.6.

Output variables are the mass flow (key MF on the *NODE PRINT or *NODE FILE card), the fluid depth (key PN — network pressure — on the *NODE PRINT card and DEPT on the *NODE FILE card) and the total temperature (key NT on the *NODE PRINT card and TT on the *NODE FILE card). These are the primary variables in the network. Internally, in network nodes, components one to three of the structural displacement field are used for the mass flow, the fluid depth and the critical depth, respectively. So their output can also be obtained by requesting U on the *NODE PRINT card. This is the only way to get the critical depth in the .dat file. In the .frd file the critical depth can be obtained by selecting HCRI on the *NODE FILE card. Notice that for liquids the total temperature virtually coincides with the static temperature (cf. previous section; recall that the wave speed in a channel with water depth 1 m is $\sqrt{10}$ m/s). If a jump occurs in the network, this is reported on the screen listing the element in which the jump takes place and its relative location within the element.

6.9.19 Three-dimensional Navier-Stokes Calculations

This option is not available in Version 2.7.

6.9.20 Substructure Generation

This procedure can be used to create the stiffness matrix of a substructure (sometimes also called a superelement) and store it in a file. A substructure consists of selected degrees of freedom of a model. It can be used in a subsequent linear analysis (this option is not available in CalculiX). In such an analysis, only the selected degrees of freedom are addressable, e.g. to apply loads or boundary conditions. The other degrees of freedom have been removed, thereby substantially reducing the size of the stiffness matrix. The retained degrees of freedom kind of constitute a new element (which explains the term superelement).

The substructure generation is triggered by the procedure card *SUBSTRUCTURE GENERATE. The degrees of freedom which should be retained can be defined by using the *RETAINED NODAL DOFS card. No transformation is allowed, consequently, the degrees of freedom apply to the global Carthesian system. Finally, the storage of the stiffness matrix is governed by the *SUBSTRUCTURE MATRIX OUTPUT card, specifying the name of the file without extension. The extension .mtx is default.

The output in the .mtx file constitutes the input one needs to use the superelement in ABAQUS. It consists of:

- a *USER ELEMENT card specifying the number of degrees of freedom involved in the substructure (misleadingly defined as "nodes").
- a list of the nodes. Each node is listed as many times as the number of its degrees of freedom in the substructure.
- for each retained degree of freedom its global direction. The format for the first degree of freedom of the substructure is just the global direction. For the subsequent degrees of freedom it consists of the number of the degree of freedom followed by the global direction
- a *MATRIX,TYPE=STIFFNESS card followed by the upper triangle (including the diagonal) of the stiffness matrix, column by column, and comma separated.

Since substructures cannot be used in CalculiX, the generation of the substructure stiffness matrix is meant to be used by other programs.

6.9.21 Electromagnetism

In CalculiX, certain types of electromagnetic calculations are possible. These include:

- electrostatic calculations: these can be performed as a special case of thermal calculations, cf. Section 6.9.13.
- magnetostatic calculations. Due to the absence of time derivatives the interaction between electric and magnetic fields drops out and the magnetic equations can be considered on their own.
- magnetic induction calculations. These are calculations without fixed electric charges and in which the displacement current can be neglected. The major industrial application for this type of calculation is inductive heating.

In this section only the last two applications are treated. The governing Maxwell equations run like (the displacement current term was dropped in Equation (265)):

$$\nabla \cdot \boldsymbol{D} = \rho \tag{262}$$

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t} \tag{263}$$

$$\nabla \cdot \boldsymbol{B} = 0 \tag{264}$$

$$\nabla \times \boldsymbol{H} = \boldsymbol{j} \tag{265}$$

where $\boldsymbol{E}$ is the electric field, $\boldsymbol{D}$ is the electric displacement field, $\boldsymbol{B}$ is the magnetic field, $\boldsymbol{H}$ is the magnetic intensity, $\boldsymbol{j}$ is the electric current density and ρ is the electric charge density. These fields are connected by the following constitutive equations:

$$\boldsymbol{D} = \epsilon \boldsymbol{E} \tag{266}$$

$$\boldsymbol{B} = \mu \boldsymbol{H} \tag{267}$$

and

$$\boldsymbol{j} = \sigma \boldsymbol{E}. \tag{268}$$

Here, ϵ is the permittivity, μ is the magnetic permeability and σ is the electrical conductivity. For the present applications ϵ and $\boldsymbol{D}$ are not needed and Equation (262) can be discarded. It will be assumed that these relationships are linear and isotropic, the material parameters, however, can be temperature dependent. So no hysteresis is considered, which basically means that only paramagnetic and diamagnetic materials are considered. So far, no ferromagnetic materials are allowed.

Due to electromagnetism, an additional basic unit is needed, the Ampère (A). All other quantities can be written using the SI-units A, m, s, kg and K, however, frequently derived units are used. An overview of these units is given in Table 17.

In what follows the references [65] and [36] have been used. In inductive heating applications the domain of interest consists of the objects to be heated (= workpiece), the surrounding air and the coils providing the current leading to the induction. It will be assumed that the coils can be considered seperately as a driving force without feedback from the system. This requires the coils to be equiped with a regulating system counteracting any external influence trying to modify the current as intended by the user.

Let us first try to understand what happens physically. In the simplest case the volume to be analyzed consists of a simply connected body surrounded by air, Figure 122. A body is simply connected if any fictitious closed loop within the body can be reduced to a point without leaving the body. For instance, a sphere is simply connected, a ring is not. The coil providing the current is located within the air. Turning on the current leads to a magnetic intensity field through Equation (265) and a magnetic field through Equation (267) everywhere, in the air and in the body. If the current is not changing in time, this constitutes the solution to the problem.

If the current is changing in time, so is the magnetic field, and through Equation (263) one obtains an electric field everywhere. This electric field generates a current by Equation (268) (called Eddy currents) in any part which is electrically conductive, i.e. generally in the body, but not in the air. This current

Table 17: Frequently used units electromagnetic applications.

symbol	meaning	unit
I	current	A
$\boldsymbol{E}$	electric field	$\frac{\mathrm{V}}{\mathrm{m}} = \frac{\mathrm{kg.m}}{\mathrm{A.s^3}}$
$\boldsymbol{D}$	electric displacement field	$\frac{\mathrm{C}}{\mathrm{m^2}} = \frac{\mathrm{A.s}}{\mathrm{m^2}}$
$\boldsymbol{B}$	magnetic field	$\mathrm{T} = \frac{\mathrm{kg}}{\mathrm{A.s^2}}$
$\boldsymbol{H}$	magnetic intensity	$\frac{\mathrm{A}}{\mathrm{m}}$
$\boldsymbol{j}$	current density	$\frac{\mathrm{A}}{\mathrm{m^2}}$
ϵ	permittivity	$\frac{\mathrm{F}}{\mathrm{m}} = \frac{\mathrm{A^2 s^4}}{\mathrm{kgm^3}}$
μ	magnetic permeability	$\frac{\mathrm{kg.m}}{\mathrm{A^2.s^2}}$
σ	electrical conductivity	$\frac{\mathrm{S}}{\mathrm{m}} = \frac{\mathrm{A^2.s^3}}{\mathrm{kg.m^3}}$
P	magnetic scalar potential	A
V	electric scalar potential	$\mathrm{V} = \frac{\mathrm{kg.m^2}}{\mathrm{A.s^3}}$
$\boldsymbol{A}$	magnetic vector potential	$\frac{\mathrm{kg.m}}{\mathrm{A.s^2}}$

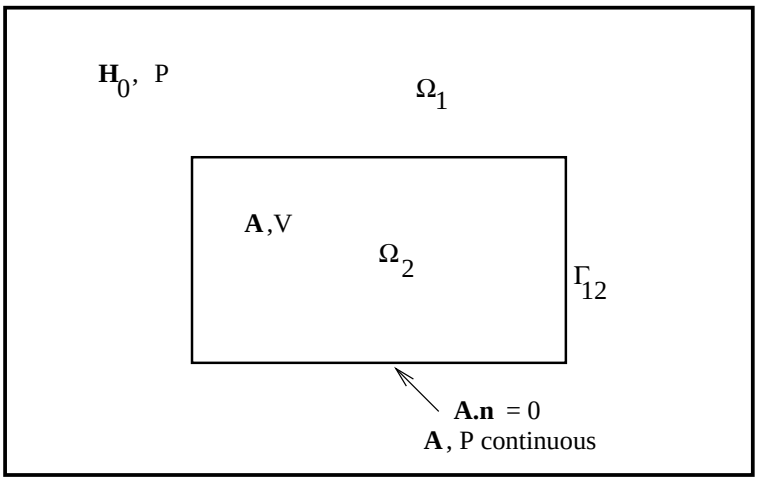


Figure 122: Electromagnetic setup for simply connected bodies

generates a magnetic intensity field by virtue of Equation (265), in a direction which is opposite to the original magnetic intenstiy field. Thus, the Eddy currents oppose the generation of the magnetic field in the body. Practically, this means that the magnetic field in the body is not built up at once. Rather, it is built up gradually, in the same way in which the temperature in a body due to heat transfer can only change gradually. As a matter of fact, both phenomena are described by first order differential equations in time. The Ohm-losses of the Eddy currents are the source of the heat generation used in industrial heat induction applications.

From these considerations one realizes that in the body (domain 2, cf. Figure 122; notice that domain 1 and 2 are interchanged compared to [65]) both the electric and the magnetic field have to be calculated, while in the air it is sufficient to consider the magnetic field only (domain 1). Therefore, in the air it is sufficient to use a scalar magnetic potential P satisfying:

$$\boldsymbol{H} = \boldsymbol{T_0} - \nabla P. \tag{269}$$

Here, $\boldsymbol{T_0}$ is the magnetic intensity due to the coil current in infinite free space. $\boldsymbol{T_0}$ can be calculated using the Biot-Savart relationships [22]. The body fields can be described using a vector magnetic potential $\boldsymbol{A}$ and a scalar electric potential V satisfying:

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}, \tag{270}$$

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t} - \nabla V. \tag{271}$$

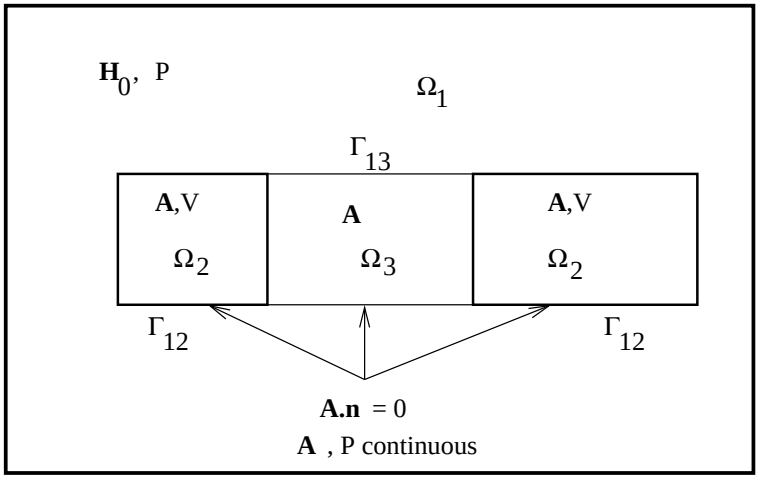


Figure 123: Electromagnetic setup for multiply connected bodies

In practice, it is convenient to set $V = \frac{\partial v}{\partial t}$, leading to

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t} - \frac{\partial \nabla v}{\partial t}. \tag{272}$$

This guarantees that the resulting matrices will be symmetric.

If the body is multiply connected, the calculational domain consists of three domains. The body (or bodies) still consist of domain 2 governed by the unknowns $\boldsymbol{A}$ and V. The air, however, has to split into two parts: one part which is such that, if added to the bodies, makes them simply connected. This is domain 3 and it is described by the vector magnetic potential $\boldsymbol{A}$. It is assumed that there are no current conducting coils in domain 3. The remaining air is domain 1 described by the scalar magnetic potential P.

In the different domains, different equations have to be solved. In domain 1 the electric field is not important, since there is no conductance. Therefore, it is sufficient to calculate the magnetic field, and only Equations (264) and (265) have to be satisfied. Using the ansatz in Equation (269), Equation (265) is automatically satiesfied, since it is satisfied by $\boldsymbol{T_0}$ and the curl of the gradient vanishes. The only equation left is (264). One arrives at the equation

$$\nabla \cdot \mu(\boldsymbol{T_0} - \nabla P) = 0. \tag{273}$$

In domain 2, Equations (263), (264) and (265) have to be satisfied, using the approach of Equations (270) and (271). Taking the curl of Equation (271)

yields Equation (263). Taking the divergence of Equation (270) yields Equation (264). Substituting Equations (270) and (271) into Equation (265) leads to:

$$\nabla \times \frac{1}{\mu}(\nabla \times \boldsymbol{A}) + \sigma \frac{\partial \boldsymbol{A}}{\partial t} + \sigma \nabla V = 0. \tag{274}$$

The magnetic vector potential $\boldsymbol{A}$ is not uniquely defined by Equation (270). The divergence of $\boldsymbol{A}$ can still be freely defined. Here, we take the Coulomb gauge, which amounts to setting

$$\nabla \cdot \boldsymbol{A} = 0. \tag{275}$$

Notice that the fulfillment of Equation (265) automatically satisfies the conservation of charge, which runs in domain 2 as

$$\nabla \cdot \boldsymbol{j} = 0, \tag{276}$$

since there is no concentrated charge. Thus, for a simply connected body we arrive at the Equations (273) (domain 1), (274) (domain 2) and (275) (domain 2). In practice, Equations (274) and (275) are frequently combined to yield

$$\nabla \times \frac{1}{\mu}(\nabla \times \boldsymbol{A}) - \nabla \frac{1}{\mu} \nabla \cdot \boldsymbol{A} + \sigma \frac{\partial \boldsymbol{A}}{\partial t} + \sigma \nabla V = 0. \tag{277}$$

This, however, is not any more equivalent to the solution of Equation (265) and consequently the satisfaction of Equation (276) has now to be requested explicitly:

$$\nabla \cdot \sigma (\frac{\partial \boldsymbol{A}}{\partial t} + \nabla V) = 0. \tag{278}$$

Consequently, the equations to be solved are now Equations (277) (domain 2), (278) (domain 2), and (273) (domain 1).

In domain 3, only Equations (264) and (265) with $\boldsymbol{j} = 0$ have to be satisfied (the coils are supposed to be in domain 1). Using the ansatz from Equation (270), Equation (264) is automatically satisfied and Equation (265) now amounts to

$$\nabla \times \frac{1}{\mu}(\nabla \times \boldsymbol{A}) - \nabla \frac{1}{\mu} \nabla \cdot \boldsymbol{A} = 0. \tag{279}$$

The boundary conditions on the interface amount to:

- continuity of the normal component of $\boldsymbol{B}$
- continuity of the tangential component of $\boldsymbol{H}$, and
- no current flow orthogonal to the boundary, or ($\boldsymbol{n_i}$ is the normal on domain i, pointing away from the domain):

$$\boldsymbol{B_1} \cdot \boldsymbol{n_1} + \boldsymbol{B_2} \cdot \boldsymbol{n_2} = 0, \tag{280}$$

$$\boldsymbol{H_1} \times \boldsymbol{n_1} + \boldsymbol{H_2} \times \boldsymbol{n_2} = 0 \tag{281}$$

and

$$\boldsymbol{j_2} \cdot \boldsymbol{n_2} = 0 \tag{282}$$

all of which have to be satisfied on Γ_{12}. In terms of the magnetic vector potential $\boldsymbol{A}$, electric scalar potential V and magnetic scalar potential P this amounts to:

$$\mu(\boldsymbol{T_0} - \nabla P) \cdot \boldsymbol{n_1} + (\nabla \times \boldsymbol{A}) \cdot \boldsymbol{n_2} = 0, \tag{283}$$

$$(\boldsymbol{T_0} - \nabla P) \times \boldsymbol{n_1} + \frac{1}{\mu_1}(\nabla \times \boldsymbol{A}) \times \boldsymbol{n_2} = 0 \tag{284}$$

and

$$(\frac{\partial \boldsymbol{A}}{\partial t} + \nabla V)_2 \cdot \boldsymbol{n_2} = 0 \tag{285}$$

on Γ_{12}. For uniqueness, the electric potential has to be fixed in one node and the normal component of $\boldsymbol{A}$ has to vanish along Γ_{12} [65]:

$$\boldsymbol{A} \cdot \boldsymbol{n_2} = 0. \tag{286}$$

To obtain the weak formulation of the above equations they are multiplied with trial functions and integrated. The trial functions will be denoted by $\delta\boldsymbol{A}, \delta V$ and δP. Starting with Equation(277) one obtains after multiplication with $\boldsymbol{\delta A}$ and taking the vector identies

$$\nabla \cdot (\boldsymbol{a} \times \boldsymbol{b}) = (\nabla \times \boldsymbol{a}) \cdot \boldsymbol{b} - \boldsymbol{a} \cdot (\nabla \times \boldsymbol{b}) \tag{287}$$

$$\nabla \cdot (\alpha \boldsymbol{a}) = \nabla\alpha \cdot \boldsymbol{a} + \alpha \nabla \cdot \boldsymbol{a} \tag{288}$$

into account (set $\boldsymbol{b} = (\nabla \times \boldsymbol{A})/\mu$ in the first vector identity):

$$\begin{aligned} &\frac{1}{\mu}(\nabla \times \delta\boldsymbol{A}) \cdot (\nabla \times \boldsymbol{A}) - \nabla \cdot (\delta\boldsymbol{A} \times \frac{1}{\mu}\nabla \times \boldsymbol{A}) + \frac{1}{\mu}(\nabla \cdot \boldsymbol{A})\nabla \cdot (\delta\boldsymbol{A}) \\ &- \nabla \cdot [\frac{1}{\mu}(\nabla \cdot \boldsymbol{A})\delta\boldsymbol{A}] + \delta\boldsymbol{A} \cdot \sigma \left(\frac{\partial \boldsymbol{A}}{\partial t} + \nabla V \right) = 0. \end{aligned} \tag{289}$$

Integrating one obtains, using Gauss' theorem (it is assumed that Ω_2 has no free boundary, i.e. no boundary not connected to Ω_1):

$$\int_{\Omega_2} \frac{1}{\mu}(\nabla \times \delta \boldsymbol{A}) \cdot (\nabla \times \boldsymbol{A}) d\Omega - \int_{\Gamma_{12}} \frac{1}{\mu}(\delta \boldsymbol{A} \times \nabla \boldsymbol{A}) \cdot \boldsymbol{n_2} dS + \int_{\Omega_2} \frac{1}{\mu}(\nabla \cdot \boldsymbol{A})(\nabla \cdot \delta \boldsymbol{A}) d\Omega - \int_{\Gamma_{12}} \frac{1}{\mu}(\nabla \cdot \boldsymbol{A}) \delta \boldsymbol{A} \cdot \boldsymbol{n_2} dS + \int_{\Omega_2} \delta \boldsymbol{A} \cdot \sigma \left(\frac{\partial \boldsymbol{A}}{\partial t} + \nabla V \right) d\Omega = 0 \tag{290}$$

The trial functions also have to satisfy the kinematic constraints. Therefore, $\delta \boldsymbol{A} \cdot \boldsymbol{n_2} = 0$ and the second surface integral is zero.

Applying the vector identity

$$(\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{n} = \boldsymbol{a} \cdot (\boldsymbol{b} \times \boldsymbol{n}) \tag{291}$$

and the boundary condition from Equation (284), the integrand of the first surface integral can be written as:

$$\begin{aligned} &\frac{1}{\mu}(\delta \boldsymbol{A} \times \nabla \times \boldsymbol{A}) \cdot \boldsymbol{n_2} = \\ &\frac{1}{\mu}\left(\delta \boldsymbol{A} \cdot [(\nabla \times \boldsymbol{A}) \times \boldsymbol{n_2}]\right) = \\ &-\delta \boldsymbol{A} \cdot [(\boldsymbol{T_0} - \nabla \boldsymbol{P}) \times \boldsymbol{n_1}]. \end{aligned} \tag{292}$$

Consequently, the integral now amounts to:

$$\int_{\Gamma_{12}} \left[-\delta \boldsymbol{A} \cdot (\boldsymbol{T_0} \times \boldsymbol{n_2}) + \delta \boldsymbol{A} \cdot (\nabla P \times \boldsymbol{n_2})\right] dS. \tag{293}$$

Applying the same vector identity from above one further arrives at:

$$\int_{\Gamma_{12}} \left[-\delta \boldsymbol{A} \cdot (\boldsymbol{T_0} \times \boldsymbol{n_2}) + \boldsymbol{n_2} \cdot (\delta \boldsymbol{A} \times \nabla P)\right] dS. \tag{294}$$

Finally, using the vector identity:

$$\boldsymbol{n_2} \cdot (\delta \boldsymbol{A} \times \nabla P) = P[\boldsymbol{n_2} \cdot (\nabla \times \delta \boldsymbol{A})] - \boldsymbol{n_2} \cdot [\nabla \times (P \delta \boldsymbol{A})] \tag{295}$$

one obtains

$$\int_{\Gamma_{12}} \{-\delta \boldsymbol{A} \cdot (\boldsymbol{T_0} \times \boldsymbol{n_2}) + P[\boldsymbol{n_2} \cdot (\nabla \times \delta \boldsymbol{A})] - \boldsymbol{n_2} \cdot [\nabla \times (P \delta \boldsymbol{A})]\} dS. \tag{296}$$

The last integral vanishes if the surface is closed due to Stokes' Theorem.

Now the second equation, Equation (278), is being looked at. After multiplication with δV it can be rewritten as:

$$\nabla \cdot \left[\delta V \sigma \left(\frac{\partial \boldsymbol{A}}{\partial t} + \nabla V \right)\right] - \nabla \delta V \cdot \sigma \left(\frac{\partial \boldsymbol{A}}{\partial t} + \nabla V \right) = 0. \tag{297}$$

After integration and application of Gauss' theorem one ends up with the last term only, due to the boundary condition from Equation (285).

Analogously, the third equation, Equation (273) leads to:

$$\nabla \cdot (\delta P \mu [\boldsymbol{T_0} - \nabla P]) - \nabla \delta P \cdot \mu (\boldsymbol{T_0} - \mu \nabla P) = 0. \tag{298}$$

After integration this leads to (on external faces of Ω_1, i.e. faces not connected to Ω_2 or Ω_3 the condition $\boldsymbol{B} \cdot \boldsymbol{n_1} = 0$ is applied) :

$$\int_{\Omega_1} \nabla \delta P \cdot \mu (\boldsymbol{T_0} - \mu \nabla P) d\Omega - \int_{\Gamma_{12}} \delta P \mu (\boldsymbol{T_0} - \nabla P] \cdot \boldsymbol{n_1} dS = 0. \tag{299}$$

Applying the boundary condition from Equation (283) leads to:

$$\int_{\Omega_1} \nabla \delta P \cdot \mu (\boldsymbol{T_0} - \mu \nabla P) d\Omega + \int_{\Gamma_{12}} \delta P (\nabla \times \boldsymbol{A}) \cdot \boldsymbol{n_2} dS = 0. \tag{300}$$

So one finally obtains for the governing equations :

$$\begin{aligned} &\int_{\Omega_2} \frac{1}{\mu} (\nabla \times \delta \boldsymbol{A}).(\nabla \times \boldsymbol{A}) d\Omega + \int_{\Omega_2} \frac{1}{\mu} (\nabla \cdot \delta \boldsymbol{A})(\nabla \cdot \boldsymbol{A} d\Omega + \\ &\int_{\Omega_2} (\delta \boldsymbol{A}) \cdot \sigma (\frac{\partial \boldsymbol{A}}{\partial t} + \nabla \frac{\partial v}{\partial t}) d\Omega + \int_{\Gamma_{12}} P (\nabla \times \delta \boldsymbol{A}) \cdot \boldsymbol{n}_2 dS \\ &= \int_{\Gamma_{12}} \delta \boldsymbol{A} \cdot (\boldsymbol{T_0} \times \boldsymbol{n}_2) dS \end{aligned} \tag{301}$$

$$\int_{\Omega_2} \nabla \delta V \cdot \sigma \left(\frac{\partial \boldsymbol{A}}{\partial t} + \nabla \frac{\partial v}{\partial t} \right) d\Omega = 0 \tag{302}$$

$$\begin{aligned} &- \int_{\Omega_1} \mu \nabla \delta P \cdot \nabla P d\Omega + \int_{\Gamma_{12}} (\delta P)(\nabla \times \boldsymbol{A}) \cdot \boldsymbol{n}_2 dS \\ &= \int_{\Omega_1} \mu \nabla \delta P \cdot \boldsymbol{T_0} d\Omega. \end{aligned} \tag{303}$$

Using the standard shape functions one arrives at (cf. Chapter 2 in [18]):

$$\sum_e \sum_{i=1}^{N} \sum_{j=1}^{N} \Bigg\{ \left[\int_{V_{0e2}} \varphi_{i,L} \frac{1}{\mu} \varphi_{j,L} \delta_{KM} dV_e \right] \delta A_{iK} A_{jM} -$$
$$\left[\int_{V_{0e2}} \varphi_{i,M} \frac{1}{\mu} \varphi_{j,K} dV_e \right] \delta A_{iK} A_{jM} +$$
$$\left[\int_{V_{0e2}} \varphi_{i,K} \frac{1}{\mu} \varphi_{j,M} dV_e \right] \delta A_{iK} A_{jM} +$$
$$\left[\int_{V_{0e2}} \varphi_i \sigma \varphi_j dV_e \delta_{KM} \right] \delta A_{iK} \frac{DA_{jM}}{t} +$$
$$\left[\int_{V_{0e2}} \varphi_i \sigma \varphi_{j,K} dV_e \right] \delta A_{iK} \frac{Dv_j}{Dt} +$$
$$\left[\int_{A_{0e12}} e_{KLM} \varphi_i \varphi_{j,L} n_{2K} dA_e \right] \delta A_{jM} P_i \Bigg\} =$$
$$- \sum_e \sum_{j=1}^{N} \left[\int_{A_{0e12}} e_{KLM} \varphi_j T_{0L} n_{2K} dA_e \right] \delta A_{jM} \tag{304}$$

$$\sum_e \sum_{i=1}^{N} \sum_{j=1}^{N} \Bigg\{ \left[\int_{V_{0e2}} \varphi_{i,K} \sigma \varphi_i dV_e \right] \delta v_j \frac{DA_{iK}}{Dt}$$
$$\left[\int_{V_{0e2}} \varphi_{i,K} \sigma \varphi_{j,K} dV_e \right] \delta v_i \frac{Dv_j}{Dt} \Bigg\} = 0 \tag{305}$$

$$\sum_e \sum_{i=1}^{N} \sum_{j=1}^{N} \Bigg\{ \left[\int_{V_{0e1}} \varphi_{i,K} \mu \varphi_{j,K} dV_e \right] \delta P_i P_j \tag{306}$$
$$\left[\int_{A_{0e12}} \varphi_i e_{KLM} \varphi_{j,L} n_{2K} dA_e \right] \delta P_i A_{jM} \Bigg\} \tag{307}$$
$$= - \sum_e \sum_i \left[\int_{V_{0e1}} \mu \varphi_{i,K} T_{0K} dV_e \right] \delta P_i. \tag{308}$$

Notice that the first two equations apply to domain 2, the last one applies to domain 1. In domain 3 only the first equation applies, in which the time dependent terms are dropped.

This leads to the following matrices:

$$[K_{AA}]_{e(iK)(jM)} = \int_{(V_{0e})_{\Omega_2}} \frac{1}{\mu} [\varphi_{i,L} \varphi_{j,L} \delta_{KM} - \varphi_{i,M} \varphi_{j,K} + \varphi_{i,K} \varphi_{j,M}] dV_e \tag{309}$$

$$[K_{AP}]_{e(jM)(i)} = \int_{(A_{0e})_{\Gamma_{12}}} e_{KLM} \varphi_i \varphi_{j,L} n_{1K} dA_e \tag{310}$$

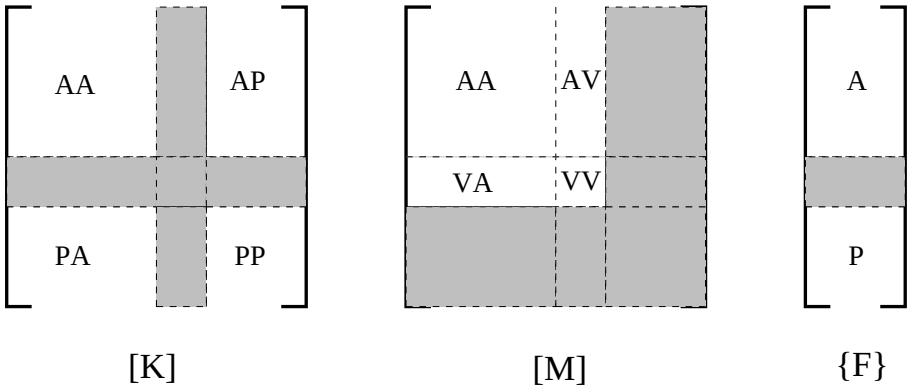


Figure 124: Nonzero parts of the governing matrices

$$[K_{PA}]_{e(i)(jM)} = \int_{(A_{0e})_{\Gamma_{12}}} e_{KLM}\varphi_i\varphi_{j,L}n_{1K}dA_e \tag{311}$$

$$[K_{PP}]_{e(i)(j)} = -\int_{(V_{0e})_{\Omega_1}} \mu\varphi_{i,K}\varphi_{j,K}dV_e \tag{312}$$

$$[M_{AA}]_{e(iK)(jM)} = \int_{(V_{0e})_{\Omega_2}} \varphi_i\sigma\varphi_j\delta_{KM}dV_e \tag{313}$$

$$[M_{Av}]_{e(iK)(j)} = \int_{(V_{0e})_{\Omega_2}} \varphi_i\sigma\varphi_{j,K}\delta_{KM}dV_e \tag{314}$$

$$[M_{vA}]_{e(j)(iK)} = \int_{(V_{0e})_{\Omega_2}} \varphi_{j,K}\sigma\varphi_i\delta_{KM}dV_e \tag{315}$$

$$[M_{vv}]_{e(i)(j)} = \int_{(V_{0e})_{\Omega_2}} \varphi_{i,K}\sigma\varphi_{i,K}\delta_{KM}dV_e \tag{316}$$

$$\{F_A\}_{e(jM)} = -\int_{(A_{0e})_{\Gamma_{12}}} e_{KLM}\varphi_j T_{0L}n_{1K}dA_e \tag{317}$$

$$\{F_P\}_{e(i)} = -\int_{(V_{0e})_{\Omega_1}} \mu\varphi_{i,K}T_{0K}dV_e \tag{318}$$

Repeated indices imply implicit summation. The $[K]$ matrices are analogous to the conductivity matrix in heat transfer analyses, the $[M]$ matrices are the counterpart of the capacity matrix. $\{F\}$ represents the force. The resulting system consists of first order ordinary differential equations in time and the corresponding matrices look like in Figure 124. Solution of this system yields the solution for $\boldsymbol{A}, vandP$ from which the magnetic field $\boldsymbol{B}$ and the electric field $\boldsymbol{E}$ can be determined using Equations (270,271).

The internal electromagnetic forces amount to:

$$\begin{aligned}\{F_A\}_{(iK)} &= [K_{AA}]_{e(iK)(jM)} \cdot \{A\}_{(jM)} + [K_{AP}]_{e(iK)(j)} \cdot \{P\}_{(j)} \\ &= \frac{1}{\mu} \int_{(V_{0e})_{\Omega_2}} [\varphi_{i,L} A_{K,L} - \varphi_{i,M} A_{M,K} + \varphi_{i,K} A_{M,M}] dV_e \\ &= - \int_{(A_{0e})_{\Gamma_{12}}} e_{KLM} \varphi_{i,L} P n_{1M} dA_e \end{aligned} \tag{319}$$

and

$$\begin{aligned}\{F\}_{(i)} &= [K_{PA}]_{e(i)(jM)} \cdot \{A\}_{(jM)} + [K_{PP}]_{e(i)(j)} \cdot \{P\}_{(j)} \\ &= \int_{(A_{0e})_{\Gamma_{12}}} \varphi_i e_{KLM} A_{M,L} n_{1K} dA_e \\ &= - \int_{(V_{0e})_{\Omega_1}} \mu \varphi_{i,K} P_{,K} dV_e. \end{aligned} \tag{320}$$

They have to be in equilibrium with the external forces.

What does the above theory imply for the practical modeling? The conductor containing the driving current is supposed to be modeled using shell elements. The thickness of the shell elements can vary. The current usually flows near the surface (skin effect), so the modeling with shell elements is not really a restriction. The current and potential in the conductor is calculated using the heat transfer analogy. This means that potential boundary conditions have to be defined as temperature, current boundary conditions as heat flow conditions. The driving current containing conductor is completely separate from the mesh used to calculate the magnetic and electric fields. Notice that the current in the driving electromagnetic coils is not supposed to be changed by the electromagnetic field it generates.

The volumetric domains of interest are $\Omega_1 \Omega_2 and \Omega_3$. These three domains represent the air, the conducting workpiece and that part of the air which, if filled with workpiece material, makes the workpiece simply connected. These three domains are to be meshed with volumetric elements. The meshes should not be connected, i.e., one can mesh these domains in a completely independent way. This also applies that one can choose the appropriate mesh density for each domain separately.

Based on the driving current the field $\boldsymbol{T_0}$ is determined in domain 1 with the Biot-Savart law. This part of the code is parallellized, since the Biot-Savart integration is calculationally quite intensive. Because of Equation (317) $\boldsymbol{T_0}$ is also determined on the external faces of domain 2 and 3 which are in contact with domain 1.

The following boundary conditions are imposed (through MPC's):
On the external faces of domain 1 which are in contact with domain 2 or domain 3:

- Calculation of $\boldsymbol{A}$ based on the external facial values in domain 2 and 3 (cf. the area integrals in $[K]$)

On the external faces of domain 2 and 3 which are in contact with domain 1:

- Calculation of P based on the external facial values in domain 1.
- Imposition of $\boldsymbol{A} \cdot \boldsymbol{n} = 0$.

On the faces between domain 2 and 3:

- Continuity of $\boldsymbol{A}$

These MPC's are generated automatically within CalculiX and have not to be taken care of by the user. Finally, the value of V has to be fixed in at least one node of domain 2. This has to be done by the user with a *BOUNDARY condition on degree of freedom 8.

The material data to be defined include:

- the electrical conductivity in the driving coils
- the magnetic permeability in the air
- the density, the thermal conductivity, the specific heat, the electrical conductivity and the magnetic permeability in the workpiece.

To this end the cards *DENSITY, *CONDUCTIVITY, *SPECIFIC HEAT, *ELECTRICAL CONDUCTIVITY, MAGNETIC PERMEABILITY can be used. In the presence of thermal radiation the *PHYSICAL CONSTANTS card is also needed.

The procedure card is *ELECTROMAGNETICS. For magnetostatic calculations the parameter MAGNETOSTATICS is to be used, for athermal electromagnetic calculations the parameter NO HEAT TRANSFER. Default is an electromagnetic calculation with heat transfer.

Available output variables are POT (the electric potential in the driving current coil) on the *NODE FILE card and ECD (electric current density in the driving current coil), EMFE (electric field in the workpiece) and EMFB (magnetic field in the air and the workpiece) on the *EL FILE card. Examples are induction.inp and induction2.inp.

6.10 Convergence criteria

To find the solution at the end of a given increment a set of nonlinear equations has to be solved. In order to do so, the Newton-Raphson method is applied, i.e. the set of equations is locally linearized and solved. If the solution does not satisfy the original nonlinear equations, the latter are again linearized at the new solution. This procedure is repeated until the solution satisfies the original nonlinear equations within a certain margin. Suppose iteration i has been performed and convergence is to be checked. Let us introduce the following quantities:

- $\bar{q}_i^\alpha$: the average flux for field α at the end of iteration i. It is defined by:

$$\bar{q}_i^\alpha = \frac{\sum_e \sum_{n_e} \sum_{k_n} |q_i^\alpha|}{\sum_e \sum_{n_e} k_n^\alpha} \tag{321}$$

  where e represents all elements, n_e all nodes belonging to a given element, k_n all degrees of freedom for field α belonging to a given node and q_i^α is the flux for a given degree of freedom of field α in a given node belonging to a given element at the end of iteration i. Right now, there are two kind of fluxes in CalculiX: the force for mechanical calculations and the concentrated heat flux for thermal calculations.

- $\tilde{q}_i^\alpha$: the iteration-average of the average flux for field α of all iterations in the present increment up to but not including iteration i.

- $r_{i,max}^\alpha$: the largest residual flux (in absolute value) of field α at the end of iteration i. For its calculation each degree of freedom is considered independently from all others:

$$r_{i,max}^\alpha = \max_e \max_{n_e} \max_{k_n} |\delta q_i^\alpha|, \tag{322}$$

  where δ denotes the change due to iteration i.

- $\Delta u_{i,max}^\alpha$: the largest change in solution (in absolute value) of field α in the present increment including iteration i. :

$$\Delta u_{i,max}^\alpha = \max_e \max_{n_e} \max_{k_n} |\Delta u_i^\alpha|, \tag{323}$$

  where Δ denotes the change due to the present increment. In mechanical calculations the solution is the displacement, in thermal calculations it is the temperature.

- $c_{i,max}^\alpha$: the largest change in solution (in absolute value) of field α in iteration i. :

$$c_{i,max}^\alpha = \max_e \max_{n_e} \max_{k_n} |\delta u_i^\alpha|. \tag{324}$$

Now, two constants c_1 and c_2 are introduced: c_1 is used to check convergence of the flux, c_2 serves to check convergence of the solution. Their values depend on whether zero flux conditions prevail or not. Zero flux is defined by

$$\bar{q}_i^\alpha \leq \epsilon^\alpha \tilde{q}_i^\alpha. \tag{325}$$

The following rules apply:

- if($\bar{q}_i^\alpha > \epsilon^\alpha \tilde{q}_i^\alpha$) (no zero flux):

  - if ($i \leq I_p[9]$) $c_1 = R_n^\alpha[0.005]$, $c_2 = C_n^\alpha[0.02]$.
  - else $c_1 = R_p^\alpha[0.02]$, $c_2 = C_n^\alpha[0.02]$.

- else (zero flux) $c_1 = \epsilon^\alpha[10^{-5}]$, $c_2 = C_\epsilon^\alpha[0.001]$

The values in square brackets are the default values. They can be changed by using the keyword card *CONTROLS. Now, convergence is obtained if

$$r_{i,max}^\alpha \leq c_1 \tilde{q}_i^\alpha \tag{326}$$

AND if, for thermal or thermomechanical calculations (*HEAT TRANSFER, *COUPLED TEMPERATURE-DISPLACEMENT or *UNCOUPLED TEMPERATURE-DISPLACEMENT), the temperature change does not exceed DELTMX,

AND at least one of the following conditions is satisfied:

- $c_{i,max}^\alpha \leq c_2 \Delta u_{i,max}^\alpha$
- $$\frac{r_{i,max}^\alpha c_{i,max}^\alpha}{min\{r_{i-1,max}^\alpha, r_{i-2,max}^\alpha\}} < c_2 \Delta u_{i,max}^\alpha. \tag{327}$$

  The left hands side is an estimate of the largest solution correction in the next iteration. This condition only applies if no gas temperatures are to be calculated (no forced convection).

- $r_{i,max}^\alpha \leq R_l^\alpha[10^{-8}]\tilde{q}_i^\alpha$. If this condition is satisfied, the increment is assumed to be linear and no solution convergence check is performed. This condition only applies if no gas temperatures are to be calculated (no forced convection).

- $\bar{q}_i^\alpha \leq \epsilon^\alpha[10^{-5}]\tilde{q}_i^\alpha$ (zero flux conditions). This condition only applies if no gas temperatures are to be calculated (no forced convection).

- $c_{i,max}^\alpha < 10^{-8}$.

If convergence is reached, and the size of the increments is not fixed by the user (no parameter DIRECT on the *STATIC, *DYNAMIC or *HEAT TRANSFER card) the size of the next increment is changed under certain circumstances:

- if($i > I_L[10]$): $d\theta = d\theta D_B[0.75]$, where $d\theta$ is the increment size relative to the step size (convergence was rather slow and the increment size is decreased).

- if($i \leq I_G[4]$) AND the same applies for the previous increment: $d\theta = d\theta D_D[1.5]$ (convergence is fast and the increment size is increased).

If no convergence is reached in iteration i, the following actions are taken:

- if, for thermomechanical calculations, the temperature change exceeds DELTMX, the size of the increment is multiplied by $\frac{\text{DELTMX}}{\text{temperature change}} D_A$ [0.85].

- if $i > I_C$[16], too many iterations are needed to reach convergence and any further effort is abandoned: CalculiX stops with an error message.

- if $i \geq I_0$[4] AND $|r^\alpha_{i,max} > 10^{-20}|$ AND $|c^\alpha_{i,max} > 10^{-20}|$ AND $r^\alpha_{i-1,max} > r^\alpha_{i-2,max}$ AND $r^\alpha_{i,max} > r^\alpha_{i-2,max}$ AND $r^\alpha_{i,max} > c_1 \tilde{q}^\alpha_i$ then:

  - if the parameter DIRECT is active, the solution is considered to be divergent and CalculiX stops with an error message.
  - else, the size of the increment is adapted according to $d\theta = d\theta D_F$[0.25] and the iteration of the increment is restarted.

- if $i \geq I_R$[8], the number of iterations x is estimated needed to reach convergence. x roughly satisfies:

$$r^\alpha_{i,max} \left(\frac{r^\alpha_{i,max}}{r^\alpha_{i-1,max}} \right)^x = R^\alpha_n \tilde{q}^\alpha_i \tag{328}$$

  from which x can be determined. Now, if

$$i + \frac{\ln\left(R^\alpha_n \frac{\tilde{q}^\alpha_i}{r^\alpha_{i,max}} \right)}{\ln\left(\frac{r^\alpha_{i,max}}{r^\alpha_{i-1,max}} \right)} > I_C[16] \tag{329}$$

  (which means that the estimated number of iterations needed to reach convergence exceeds I_C) OR $i = I_C$, the increment size is adapted according to $d\theta = d\theta D_C$[0.5] and the iteration of the increment is restarted unless the parameter DIRECT was selected. In the latter case the increment is not restarted and the iterations continue.

- if none of the above applies iteration continues.

6.11 Loading

All loading, except residual stresses, must be specified within a step. Its magnitude can be modified by a time dependent amplitude history using the *AMPLITUDE keyword. This makes sense for nonlinear static, nonlinear dynamic, modal dynamic and steady state dynamics procedures only. Default loading history is a ramp function for *STATIC procedures and step loading for *DYNAMIC and *MODAL DYNAMIC procedures.

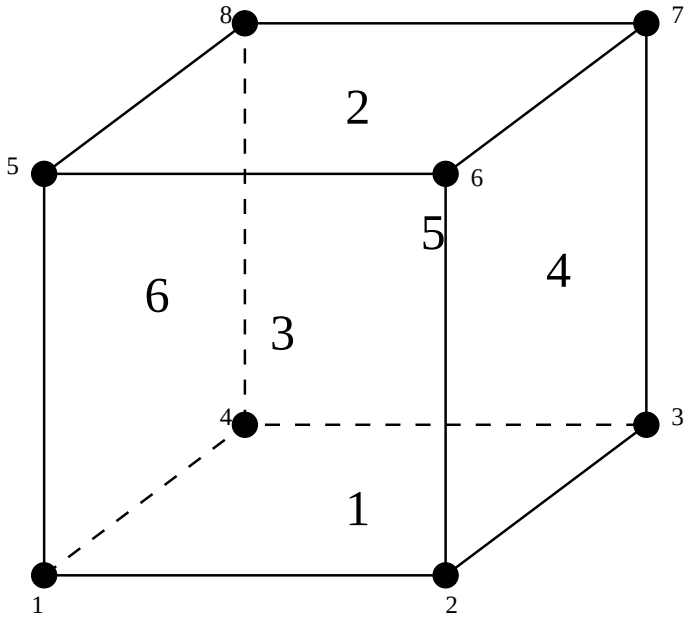


Figure 125: Face numbering for hexahedral elements

6.11.1 Point loads

Point loads are applied to the nodes of the mesh by means of the *CLOAD key word. Applying a point load at a node in a direction for which a point load was specified in a previous step replaces this point load, otherwise it is added. The parameter OP=NEW on the *CLOAD card removes all previous point loads. It takes only effect for the first *CLOAD card in a step. A buckling step always removes all previous loads.

6.11.2 Facial distributed loading

Distributed loading is triggered by the *DLOAD card. Facial distributed loads are entered as pressure loads on the element faces, which are for that purpose numbered according to Figures 125, 126 and 127.

Thus, for hexahedral elements the faces are numbered as follows:

- Face 1: 1-2-3-4
- Face 2: 5-8-7-6
- Face 3: 1-5-6-2
- Face 4: 2-6-7-3
- Face 5: 3-7-8-4

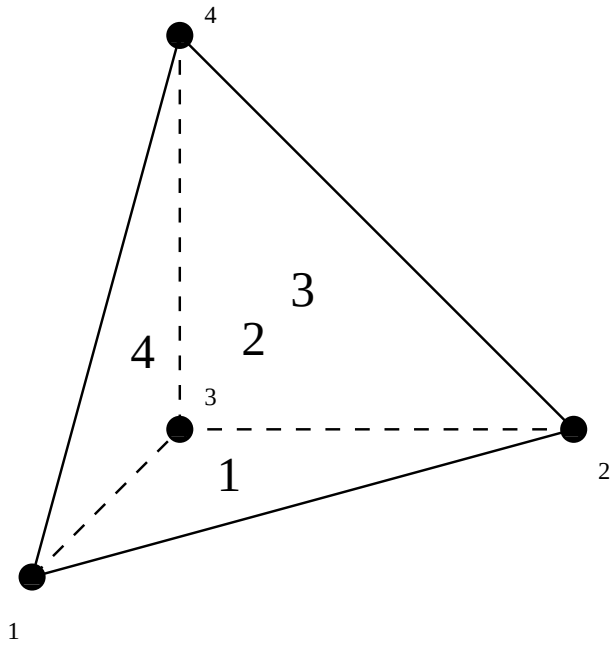


Figure 126: Face numbering for tetrahedral elements

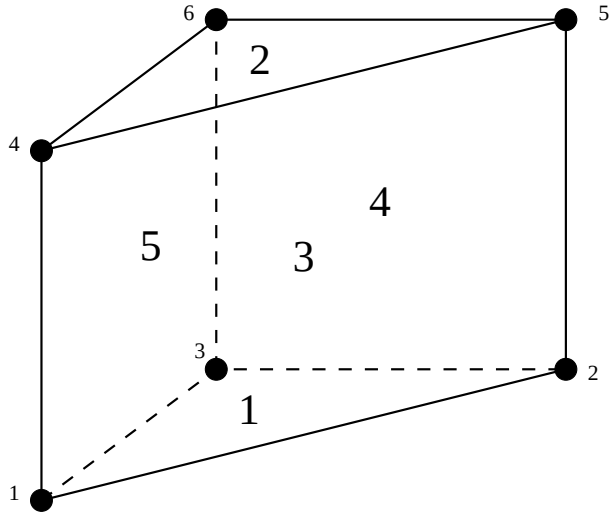


Figure 127: Face numbering for wedge elements

- Face 6: 4-8-5-1

for tetrahedral elements:

- Face 1: 1-2-3
- Face 2: 1-4-2
- Face 3: 2-4-3
- Face 4: 3-4-1

for wedge elements:

- Face 1: 1-2-3
- Face 2: 4-5-6
- Face 3: 1-2-5-4
- Face 4: 2-3-6-5
- Face 5: 3-1-4-6

for quadrilateral plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-4
- Face 4: 4-1

for triangular plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-1

for beam elements:

- Face 1: pressure in 1-direction
- Face 2: pressure in 2-direction

For shell elements no face number is needed since there is only one kind of loading: pressure in the direction of the normal on the shell.

Applying a pressure to a face for which a pressure was specified in a previous step replaces this pressure. The parameter OP=NEW on the *DLOAD card removes all previous distributed loads. It only takes effect for the first *DLOAD card in a step. A buckling step always removes all previous loads.

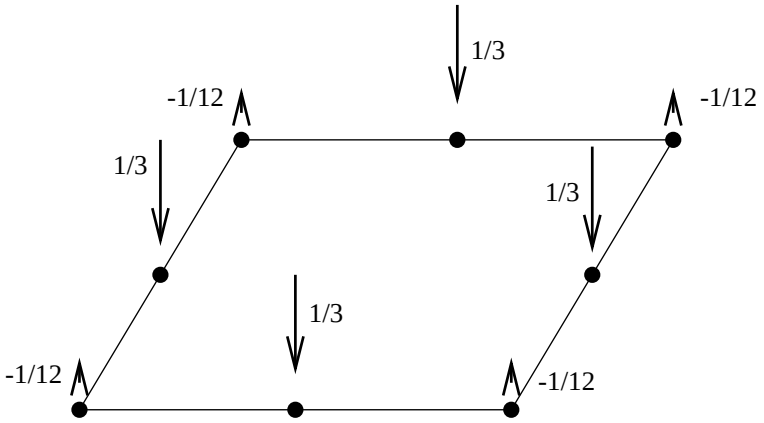


Figure 128: Equivalent nodal forces for a face of a C3D20(R) element

In a large deformation analysis the pressure is applied to the deformed face of the element. Thus, if you pull a rod with a constant pressure, the total force will decrease due to the decrease of the cross-sectional area of the rod. This effect may or may not be intended. If not, the pressure can be replaced by nodal forces. Figures 128 and 129 show the equivalent forces for a unit pressure applied to a face of a C3D20(R) and C3D10 element. Notice that the force is zero (C3D10) or has the opposite sign (C3D20(R)) for quadratic elements. For the linear C3D8(R) elements, the force takes the value 1/4 in each node of the face.

6.11.3 Centrifugal distributed loading

Centrifugal loading is selected by the *DLOAD card, together with the CENTRIF label. Centrifugal loading is characterized by its magnitude (defined as the rotational speed square ω^2) and two points on the rotation axes. To obtain the force per unit volume the centrifugal loading is multiplied by the density. Consequently, the material density is required. The parameter OP=NEW on the *DLOAD card removes all previous distributed loads. It only takes effect for the first *DLOAD card in a step. A buckling step always removes all previous loads.

6.11.4 Gravity distributed loading

Gravity loading with known gravity vector is selected by the *DLOAD card, together with the GRAV label. It is characterized by the vector representing the acceleration. The material density is required. Several gravity load cards can appear in one and the same step, provided the element set and/or the direction of the load varies (else, the previous gravity load is replaced). The parameter OP=NEW on the *DLOAD card removes all previous distributed

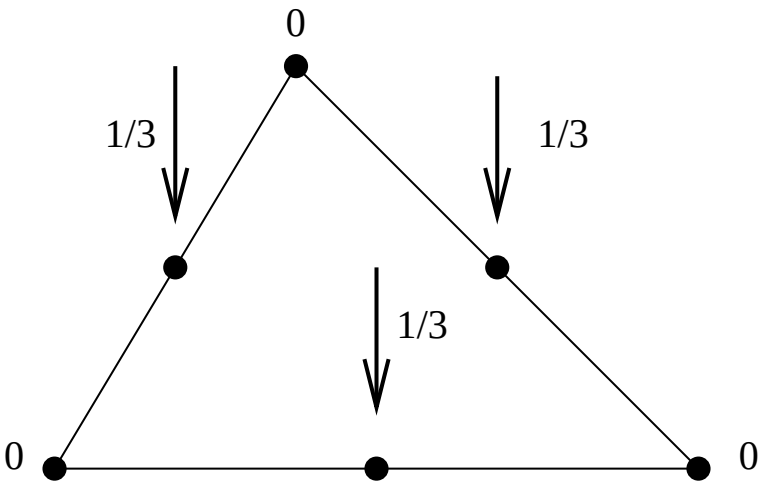


Figure 129: Equivalent nodal forces for a face of a C3D10 element

loads. It only takes effect for the first *DLOAD card in a step. A buckling step always removes all previous loads.

General gravity loading, for which the gravity vector is calculated by the momentaneous mass distribution is selected by the *DLOAD card, together with the NEWTON label. For this type of loading to make sense all elements must be assigned a NEWTON type label loading, since only these elements are taken into account for the mass distribution calculation. This type of loading requires the material density (*DENSITY) and the universal gravitational constant (*PHYSICAL CONSTANTS). It is typically used for the calculation of orbits and automatically triggers a nonlinear calculation. Consequently, it can only be used in the *STATIC, *VISCO, *DYNAMIC or *COUPLED TEMPERATURE-DISPLACEMENT step and not in a *FREQUENCY, *BUCKLE, *MODAL DYNAMIC or *STEADY STATE DYNAMICS step. It's use in a *HEAT TRANSFER step is possible, but does not make sense since mechanical loading is not taken into account in a pure heat transfer analysis.

6.11.5 Temperature loading in a mechanical analysis

Temperature loading is triggered by the keyword *TEMPERATURE. Specification of initial temperatures (*INITIAL CONDITIONS, TYPE=TEMPERATURE) and expansion coefficients (*EXPANSION) is required. The temperature is specified at the nodes. Redefined temperatures replace existing ones.

6.11.6 Initial(residual) stresses

In each integration point of an element a residual stress tensor can be specified by the keyword *INITIAL CONDITIONS, TYPE=STRESS. The residual stress should be defined before the first *STEP card.

6.11.7 Concentrated heat flux

Concentrated heat flux can be defined in nodes by using the *CFLUX card. The units are those of power, flux entering the body is positive, flux leaving the body is negative.

6.11.8 Distributed heat flux

Distributed heat flux can be defined on element sides by using the *DFLUX card. The units are those of power per unit of area, flux entering the body is positive, flux leaving the body is negative. Nonuniform flux can be defined by using the subroutine dflux.f.

In the absence of a *DFLUX card for a given element face, no distributed heat flux will be applied to this face. This seems reasonable, however, this only applies to solid structures. Due to the iterative way in which fluid dynamics calculations are performed an external element face in a CFD calculation exhibits no heat flux only if a *DFLUX card was defined for this surface with a heat flux value of zero.

6.11.9 Convective heat flux

Convective heat flux is a flux depending on the temperature difference between the body and the adjacent fluid (liquid or gas) and is triggered by the *FILM card. It takes the form

$$q = h(T - T_0) \tag{330}$$

where q is the a flux normal to the surface, h is the film coefficient, T is the body temperature and T_0 is the environment fluid temperature (also called sink temperature). Generally, the sink temperature is known. If it is not, it is an unknown in the system. Physically, the convection along the surface can be forced or free. Forced convection means that the mass flow rate of the adjacent fluid (gas or liquid) is known and its temperature is the result of heat exchange between body and fluid. This case can be simulated by CalculiX by defining network elements and using the *BOUNDARY card for the first degree of freedom in the midside node of the element. Free convection, for which the mass flow rate is a n unknown too and a result of temperature differences, cannot be simulated.

6.11.10 Radiative heat flux

Radiative heat flux is a flux depending on the temperature of the body and is triggered by the *RADIATE card. No external medium is needed. If other bodies are present, an interaction takes place. This is called cavity radiation. Usually, it is not possible to model all bodies in the environment. Then, a

homogeneous environmental body temperature can be defined. In that case, the radiative flux takes the form

$$q = \epsilon(\theta^4 - \theta_0^4) \tag{331}$$

where q is a flux normal to the surface, ϵ is the emissivity, θ is the absolute body temperature (Kelvin) and θ_0 is the absolute environment temperature (also called sink temperature). The emissivity takes values between 0 and 1. A zero value applied to a body with no absorption nor emission and 100 % reflection. A value of 1 applies to a black body. The radiation is assumed to be diffuse (independent of the direction of emission) and gray (independent of the emitted wave length).

If other bodies are present, the radiative interaction is taken into account and viewfactors are calculated if the user selects the appropriate load label.

6.12 Error estimators

6.12.1 Zienkiewicz-Zhu error estimator

The Zienkiewicz-Zhu error estimator [80], [81] tries to estimate the error made by the finite element discretization. To do so, it calculates for each node an improved stress and defines the error as the difference between this stress and the one calculated by the standard finite element procedure.

The stress obtained in the nodes using the standard finite element procedure is an extrapolation of the stresses at the integration points [18]. Indeed, the basic unknowns in mechanical calculations are the displacements. Differentiating the displacements yields the strains, which can be converted into stresses by means of the appropriate material law. Due to the numerical integration used to obtain the stiffness coefficients, the strains and stresses are most accurate at the integration points. The standard finite element procedure extrapolates these integration point values to the nodes. The way this extrapolation is done depends on the kind of element [18]. Usually, a node belongs to more than one element. The standard procedure averages the stress values obtained from each element to which the node belongs.

To determine a more accurate stress value at the nodes, the Zienkiewicz-Zhu procedure starts from the stresses at the reduced integration points. This applies to quadratic elements only, since only for these elements a reduced integration procedure exists (for element types different from C3D20R the ordinary integration points are taken instead) . The reduced integration points are superconvergent points, i.e. points at which the stress is an order of magnitude more accurate than in any other point within the element [7]. To improve the stress at a node an element patch is defined, usually consisting of all elements to which the nodes belongs. However, at boundaries and for tetrahedral elements this patch can contain other elements too. Now, a polynomial function is defined consisting of the monomials used for the shape function of the elements at stake. Again, to improve the accuracy, other monomials may be considered

as well. The coefficients of the polynomial are defined such that the polynomial matches the stress as well as possible in the reduced integration points of the patch (in a least squares sense). Finally, an improved stress in the node is obtained by evaluating this polynomial. This is done for all stress components separately. For more details on the implementation in CalculiX the user is referred to [51].

In CalculiX one can obtain the improved CalculiX-Zhu stress by selecting ZZS underneath the *EL FILE keyword card. It is available for tetrahedral and hexahedral elements. In a node belonging to tetrahedral, hexahedral and any other type of elements, only the hexahedral elements are used to defined the improved stress, if the node does not belong to hexahedral elements the tetrahedral elements are used, if any.

6.12.2 Extrapolation error estimator

A different error estimator is based on the discontinuities which arise by extrapolating the stress values at the integration points to the nodes. It is triggered by selecting ERR underneath the *EL FILE keyword card.

A node usually belongs to several elements. The stresses are available (and most accurate) at the integration points of these elements. To obtain stress values at the nodes, CalculiX extrapolates the stress tensor at the integration points to the nodes. If a node belongs to n elements, one obtains in this way n different stress tensors at one and the same node. The final stress tensor at the node is obtained by taking the mean of all these stress tensors [18].

If the mesh is fine, the difference between these stress tensors should not be very large. Conversely, large differences may point to inaccurate results. This property is used to obtain an error estimate based on the worst principal stress and the von Mises stress (the worst principal stress is the principal stress the absolute value of which is larger than the absolute value of the other two principal stresses).

The n stress tensors at one and the same node lead to n different worst principal stress values. The standard deviation of these values is stored in PSTD. In the same way the n von Mises stresses can be dealt with: VMSTD is the standard deviation of the Von Mises stresses of all extrapolated stress tensors. PSTD and VMSTD can be considered as an indicator for the size of the error.

For heat transfer a similar error estimator was coded for the heat flux. It is triggered by selecting HER underneath the *EL FILE keyword card. It represents the standard deviation of the size of all extrapolated heat flux vectors.

6.13 Output variables

Output is provided with the commands *NODE FILE and *EL FILE in the .frd file (ASCII), with the commands *NODE OUTPUT and *ELEMENT OUTPUT in the .frd file (binary) and with the commands *NODE PRINT and *EL PRINT in the .dat file (ASCII). Binary .frd files are much shorter and can be faster read

by CalculiX GraphiX. Nodal variables (selected by the *NODE FILE, *NODE OUTPUT and *NODE PRINT keywords) are always stored at the nodes. Element variables (selected by the *EL FILE, *ELEMENT OUTPUT and *ELEMENT PRINT keywords) are stored at the integration points in the .dat file and at the nodes in the .frd file. Notice that element variables are more accurate at the integration points. The values at the nodes are extrapolated values and consequently less accurate. For example, the von Mises stress and the equivalent plastic strain at the integration points have to lie on the stress-strain curve defined by the user underneath the *PLASTIC card, the extrapolated values at the nodes do not have to.

In fluid networks interpolation is used to calculate the nodal values at nodes in which they are not defined. Indeed, due to the structure of a network element the total temperature, the static temperature and the total pressure are determined at the end nodes, whereas the mass flow is calculated at the middle nodes. Therefore, to guarantee a continuous representation in the .frd file the values of the total temperature, the static temperature and the total pressure at the middle nodes are interpolated from their end node values and the end node values of the mass flow are determined from the neighboring mid-node values. This is not done for .dat file values (missing values are in that case zero).

A major different between the FILE and PRINT requests is that the PRINT requests HAVE TO be accompanied by a set name. Consequently, the output can be limited to a few nodes or elements. The output in the .frd file can but does not have to be restricted to subsets. If no node set is selected by using the NSET parameter (both for nodal and element values, since output in the .frd file is always at the nodes) output is for the complete model.

The following output variables are available:

Table 18: List of output variables.

variable	meaning	type	.frd file	.dat file
U	displacement	nodal	x	x
PU	magnitude and phase of displacement	nodal	x	
MAXU	worst displacement orthogonal to a given vector in cyclic symmetric frequency calculations	nodal	x	
NT	structural temperature total temperature in a network	nodal	x	x
PNT	magnitude and phase of temperature	nodal	x	
TT	total temperature in a gas network	nodal	x	
TS	static temperature in a network	nodal	x	x
TTF	total temperature in a 3D fluid	nodal	x	x
TSF	static temperature in a 3D fluid	nodal	x	x
RF	reaction force	nodal	x	x

Table 18: (continued)

variable	meaning	type	.frd file	.dat file
RFL	reaction flux	nodal	x	x
PT	total pressure in a gas network	nodal	x	
PS	static pressure in a liquid network	nodal	x	x
PN	network pressure (generic term for any of the above)	nodal		x
PTF	total pressure in a 3D fluid	nodal	x	x
PSF	static pressure in a 3D fluid	nodal	x	x
CP	pressure coefficient in a compressible 3D fluid	nodal	x	x
DEPT	fluid depth in a channel network	nodal	x	
HCRI	critical depth in a channel network	nodal	x	
MF	mass flow in a network	nodal	x	x
V	velocity of a structure	nodal	x	x
VF	velocity in a 3D fluid	nodal	x	x
MACH	Mach number in a compressible 3D fluid	nodal	x	x
S	Cauchy stress (structure)	element	x	x
SF	total stress (3D fluid)	element	x	
SVF	viscous stress (3D fluid)	element	x	x
ZZS	Zienkiewicz-Zhu stress	element	x	
PHS	magnitude and phase of stress	element	x	
MAXS	worst principal stress in cyclic symmetric frequency calculations	element	x	
HFL	heat flux in a structure	element	x	x
HFLF	heat flux in a 3D fluid	element	x	x
E	Lagrange strain	element	x	x
MAXE	worst principal strain in cyclic symmetric frequency calculations	element	x	
PEEQ	equivalent plastic strain	element	x	x
ENER	internal energy	element	x	x
SDV	internal variables	element	x	x
ELSE	internal energy	whole element		x
ELKE	kinetic energy	whole element		x
EVOL	volume	whole element		x
DRAG	stress on surface	surface		x
FLUX	flux through surface	surface		x
POT	electric potential	nodal	x	
ECD	electric current density	element	x	
EMFE	electric field	element	x	

Table 18: (continued)

variable	meaning	type	.frd file	.dat file
EMFB	magnetic field	element	x	

7 Input deck format

This section describes the input of CalculiX.

The jobname is defined by the argument after the -i flag on the command line. When starting CalculiX, it will look for an input file with the name jobname.inp. Thus, if you called the executable "CalculiX" and the input deck is "beam.inp" then the program call looks like

```
CalculiX -i beam
```

The -i flag can be dropped provided the jobname follows immediately after the CalculiX call.

CalculiX will generate an output file with the name jobname.dat and an output file with the name jobname.frd. The latter can be viewed with cgx.

If the step is a *FREQUENCY step or a *HEAT TRANSFER,FREQUENCY step and the parameter STORAGE=YES is activated, CalculiX will generate a binary file containing the eigenfrequencies, the eigenmodes, the stiffness and the mass matrix with the name jobname.eig. If the step is a *MODAL DYNAMIC or *STEADY STATE DYNAMICS step, CalculiX will look for a file with that name. If any of the files it needs does not exist, an error message is generated and CalculiX will stop.

The input deck basically consists of a set of keywords, followed by data required by the keyword on lines underneath the keyword. The keywords can be accompanied by parameters on the same line, separated by a comma. If the parameters require a value, an equality sign must connect parameter and value. Blanks in the input have no significance and can be inserted as you like. The keywords and any other alphanumeric information can be written in upper case, lower case, or any mixture. The input deck is case insensitive: internally, all alphanumeric characters are changed into upper case. The data do not follow a fixed format and are to be separated by a comma. A line can only contain as many data as dictated by the keyword definition. The maximum length for user-defined names, e.g. for materials or sets, is 80 characters, unless specified otherwise.The structure of an input deck consists of geometric, topological and material data before the first step definition, and loading data (mechanical, thermal, or prescribed displacements) in one or more subsequent steps. The user must make sure that all data are given in consistent units (the units do not appear in the calculation).

A keyword can be of type step or model definition. Model Definition cards must be used before the first *STEP card. Step keywords can only be used

within a step. Among the model definition keywords, the material ones occupy a special place: they define the properties of a material and should be grouped together following a *MATERIAL card.

Node and element sets can share the same name. Internally, the names are switched to upper case and a 'N' is appended after the name of a node set and a 'E' after the name of an element set. Therefore, set names printed in error or warning messages will be discovered to be written in upper case and to have a 'N' or 'E' appended.

Keyword cards in alphabetical order:

7.1 *AMPLITUDE

Keyword type: step or model definition

This option may be used to specify an amplitude history versus time. The amplitude history should be given in pairs, each pair consisting of a value of the reference time and the corresponding value of the amplitude or by user subroutine uamplitude.f.

There are two optional parameters TIME and USER and one required parameter NAME.If the parameter TIME=TOTAL TIME is used the reference time is the total time since the start of the calculation, else it is the local step time. Use as many pairs as needed, maximum four per line.

The parameter USER indicates that the amplitude history versus time was implemented in user subroutine uamplitude.f. No pair data is required.

The parameter NAME, specifying a name for the amplitude so that it can be used in loading definitions (*BOUNDARY, *CLOAD, *DLOAD and *TEMPERATURE) is required (maximum 80 characters).

In each step, the local step time starts at zero. Its upper limit is given by the time period of the step. This time period is specified on the *STATIC, *DYNAMIC or *MODAL DYNAMIC keyword card. The default step time period is 1.

In *STEADY STATE DYNAMICS steps the time is replaced by frequency, i.e. the *AMPLITUDE is interpreted as amplitude versus frequency (in cycles/time).

The total time is the time accumulated until the beginning of the actual step augmented by the local step time. In *STEADY STATE DYNAMICS procedures total time coincides with frequency (in cycles/time).

The loading values specified in the loading definitions (*BOUNDARY, *CLOAD, *DLOAD and *TEMPERATURE) are reference values. If an amplitude is selected in a loading definition, the actual load value is obtained by multiplying the reference value with the amplitude for the actual (local step or total) time. If no amplitude is specified, the actual load value depends on the procedure: for a *STATIC procedure, ramp loading is assumed connecting the load value at the end of the previous step (0 if there was none) to the reference value at the end of the present step in a linear way. For *DYNAMIC and *MODAL DYNAMIC procedures, step loading is assumed, i.e. the actual load equals the reference load for all time instances within the step. Reference loads which are

not changed in a new step remain active, their amplitude description, however, becomes void, unless the TIME=TOTAL TIME parameter is activated. Beware that at the end of a step, all reference values for which an amplitude was specified are replaced by their actual values at that time.

Notice that no different amplitude definitions are allowed on different degrees of freedom in one and the same node if a non-global coordinate system applied to that node. For instance, if you define a cylindrical coordinate system for a node, the amplitude for a force in radial direction has to be the same as for the tangential and axial direction.

First line:

- *AMPLITUDE
- Enter the required parameter.

Following line, using as many entries as needed (unless the parameter USER was selected):

- Time.
- Amplitude.
- Time.
- Amplitude.
- Time.
- Amplitude.
- Time.
- Amplitude.

Repeat this line if more than eight entries (four data points) are needed.

`Example:`

```
*AMPLITUDE,NAME=A1
0.,0.,10.,1.
```

defines an amplitude function with name A1 taking the value 0. at t=0. and the value 1. at t=10. The time used is the local step time.

Example files: beamdy1, beamnldy.

7.2 *BEAM GENERAL SECTION

Keyword type: model definition

This option is used to assign material properties to beam elements with a cross section which is neither rectangular nor elliptical. For the available beam general sections, please consult Section 6.3. Right now, only a pipe section is coded.

Notice that internally beam general sections are expanded into beams with a rectangular cross section (this is also the way in which the beam is stored in the .frd-file and is visualized in the postprocessor. The actual cross section is taken into account by appropriate placement of the integration points). The rectangular cross section is the smallest section completely covering the beam general section. For instance, for a pipe section the expanded section is square with side length equal to the outer diameter.

The parameters ELSET, MATERIAL and SECTION are required, the parameters ORIENTATION, OFFSET1 and OFFSET2 are optional. The parameter ELSET defines the beam element set to which the material specified by the parameter MATERIAL applies. The parameter ORIENTATION allows to assign local axes to the element set. If activated, the material properties are applied to the local axis. This is only relevant for non isotropic material behavior.

The parameter SECTION defines the cross section of the beam and takes the value PIPE for a pipe cross section. It is defined by its outer radius (first parameter) and its thickness (second parameter).

The OFFSET1 and OFFSET2 parameters indicate where the axis of the beam is in relation to the reference line defined by the line representation given by the user. The index 1 and 2 refer to the local axes of the beam which are perpendicular to the local tangent. To use the offset parameters direction the local directions must be defined. This is done by defining local direction 1 on the third line of the present keyword card. The unit of the offset is the thickness of the beam in the direction of the offset. Thus, OFFSET1=0 means that in 1-direction the reference line is the axis of the shell, OFFSET2=0.5 means that in 2-direction the reference line is the top surface of the beam. The offset can take any real value and allows to construct beam of nearly arbitrary cross section and the definition of composite beams.

First line:

- *BEAM GENERAL SECTION
- Enter any needed parameters.

Second line:

- first parameter
- second parameter

Third line:

- global x-coordinate of a unit vector in 1-direction (default:0)
- global y-coordinate of a unit vector in 1-direction (default:0)
- global z-coordinate of a unit vector in 1-direction (default:-1)

Example:

```
*BEAM GENERAL SECTION,MATERIAL=EL,ELSET=Eall,SECTION=PIPE
.11,.01
1.,0.,0.
```

assigns material EL to all elements in (element) set Eall. The section of the beam is a pipe section with outer radius 0.11 and thickness 0.01.

Example files: simplebeampipe1,simplebeampipe2,simplebeampipe3,simplebeampipe4.

7.3 *BEAM SECTION

Keyword type: model definition

This option is used to assign material properties to beam element sets. The parameters ELSET, MATERIAL and SECTION are required, the parameters ORIENTATION, OFFSET1 and OFFSET2 are optional. The parameter ELSET defines the shell element set to which the material specified by the parameter MATERIAL applies. The parameter ORIENTATION allows to assign local axes to the element set. If activated, the material properties are applied to the local axis. This is only relevant for non isotropic material behavior.

The parameter SECTION defines the cross section of the beam and can take the value RECT for a rectangular cross section and CIRC for an elliptical cross section. A rectangular cross section is defined by its thickness in two perpendicular directions, an elliptical cross section is defined by the length of its principal axes. These directions are defined by specifying direction 1 on the third line of the present keyword card

The OFFSET1 and OFFSET2 parameters indicate where the axis of the beam is in relation to the reference line defined by the line representation given by the user. The index 1 and 2 refer to the local axes of the beam which are perpendicular to the local tangent. To use the offset parameters direction the local directions must be defined. This is done by defining local direction 1 on the third line of the present keyword card. The unit of the offset is the thickness of the beam in the direction of the offset. Thus, OFFSET1=0 means that in 1-direction the reference line is the axis of the shell, OFFSET2=0.5 means that in 2-direction the reference line is the top surface of the beam. The offset can take any real value and allows to construct beam of nearly arbitrary cross section and the definition of composite beams.

First line:

- *BEAM SECTION

- Enter any needed parameters.

Second line:

- thickness in 1-direction
- thickness in 2-direction

Third line:

- global x-coordinate of a unit vector in 1-direction (default:0)
- global y-coordinate of a unit vector in 1-direction (default:0)
- global z-coordinate of a unit vector in 1-direction (default:-1)

Example:

```
*BEAM SECTION,MATERIAL=EL,ELSET=Eall,OFFSET1=-0.5,SECTION=RECT
3.,1.
1.,0.,0.
```

assigns material EL to all elements in (element) set Eall. The reference line is in 1-direction on the back surface, in 2-direction on the central surface. The thickness in 1-direction is 3 unit lengths, in 2-direction 1 unit length. The 1-direction is the global x-axis.

Example files: beamcom, beammix, shellbeam, swing.

7.4 *BOUNDARY

Keyword type: step or model definition

This option is used to prescribe boundary conditions. This includes:

- temperature, displacements and rotations for structures
- total temperature, mass flow and total pressure for gas networks
- temperature, mass flow and static pressure for liquid networks
- temperature, mass flow and fluid depth for channels

For liquids and structures the total and static temperature virtually coincide, therefore both are represented by the term temperature.

The following degrees of freedom are being used:

- for structures:
  - 1: translation in the local x-direction
  - 2: translation in the local y-direction

  - 3: translation in the local z-direction
  - 4: rotation about the local x-axis (only for nodes belonging to beams or shells)
  - 5: rotation about the local y-axis (only for nodes belonging to beams or shells)
  - 6: rotation about the local z-axis (only for nodes belonging to beams or shells)
  - 11: temperature

- for gas networks:
  - 1: mass flow
  - 2: total pressure
  - 11: total temperature

- for liquid networks:
  - 1: mass flow
  - 2: static pressure
  - 11: temperature

- for liquid channels:
  - 1: mass flow
  - 2: fluid depth
  - 11: temperature

If no *TRANSFORM card applied to the node at stake, the local directions coincide with the global ones. Notice that a *TRANSFORM card is not allowed for nodes in which boundary conditions are applied to rotations.

Optional parameters are OP, AMPLITUDE, TIME DELAY, LOAD CASE, USER, MASS FLOW, FIXED, SUBMODEL and STEP. OP can take the value NEW or MOD. OP=MOD is default and implies that previously prescribed displacements remain active in subsequent steps. Specifying a displacement in the same node and direction for which a displacement was defined in a previous step replaces this value. OP=NEW implies that previously prescribed displacements are removed. If multiple *BOUNDARY cards are present in a step this parameter takes effect for the first *BOUNDARY card only.

The AMPLITUDE parameter allows for the specification of an amplitude by which the boundary values are scaled (mainly used for nonlinear static and dynamic calculations). This only makes sense for nonzero boundary values. Thus, in that case the values entered on the *BOUNDARY card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference value is replaced by the actual value at that time. In subsequent steps this value is kept constant

unless it is explicitly redefined or the amplitude is defined using TIME=TOTAL TIME in which case the amplitude keeps its validity.

The TIME DELAY parameter modifies the AMPLITUDE parameter. As such, TIME DELAY must be preceded by an AMPLITUDE name. TIME DELAY is a time shift by which the AMPLITUDE definition it refers to is moved in positive time direction. For instance, a TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The TIME DELAY parameter must only appear once on one and the same keyword card.

The LOAD CASE parameter is only active in *STEADY STATE DYNAMICS calculations. LOAD CASE = 1 means that the loading is real or in-phase. LOAD CASE = 2 indicates that the load is imaginary or equivalently phase-shifted by 90°. Default is LOAD CASE = 1.

If the USER parameter is selected the boundary values are determined by calling the user subroutine uboun.f, which must be provided by the user. This applies to all nodes listed beneath the *BOUNDARY keyword. Any boundary values specified behind the degrees of freedom are not taken into account. If the USER parameter is selected, the AMPLITUDE parameter has no effect and should not be used.

The MASS FLOW parameter specifies that the *BOUNDARY keyword is used to define mass flow rates in convective problems. A mass flow rate can only be applied to the first degree of freedom of the midside node of network elements.

Next, the FIXED parameter freezes the deformation from the previous step, or, if there is no previous step, sets it to zero.

Finally, the SUBMODEL parameter specifies that the displacements in the nodes listed underneath will be obtained by interpolation from a global model. To this end these nodes have to be part of a *SUBMODEL,TYPE=NODE card. On the latter card the result file (frd file) of the global model is defined. The use of the SUBMODEL parameter requires the STEP parameter, specifying the step in the global model which will be used for the interpolation. Notice that the displacements interpolated from the global model are not transformed, no matter what coordinate system is applied to the nodes in the submodel. Consequently, if the displacements of the global model are stored in a local coordinate system, this local system also applies to the submodel nodes in which these displacements are interpolated. One could say that the submodel nodes in which the displacements of the global model are interpolated, inherit the coordinate system in which the displacements of the global model were stored.

A distinction is made whether the conditions are homogeneous (fixed conditions), inhomogeneous (prescribed displacements) or of the submodel type.

7.4.1 Homogeneous Conditions

Homogeneous conditions should be placed before the first *STEP keyword card.

First line:

- *BOUNDARY
- Enter any needed parameters and their value.

Following line:

- Node number or node set label
- First degree of freedom constrained
- Last degree of freedom constrained. This field may be left blank if only one degree of freedom is constrained.

Repeat this line if needed.

Example:

```
*BOUNDARY
73,1,3
```

fixes the degrees of freedom one through three (global if no transformation was defined for node 73, else local) of node 73.

Example files: achteld.

7.4.2 Inhomogeneous Conditions

Inhomogeneous conditions can be defined between a *STEP card and an *END STEP card only.

First line:

- *BOUNDARY
- Enter any needed parameters and their value.

Following line:

- Node number or node set label
- First degree of freedom constrained
- Last degree of freedom constrained. This field may be left blank if only one degree of freedom is constrained.
- Actual magnitude of the prescribed displacement

Repeat this line if needed.

Example:

```
*BOUNDARY
Nall,2,2,.1
```

assigns to degree of freedom two of all nodes belonging to node set Nall the value 0.1.

Example:

```
*BOUNDARY,MASS FLOW
73,1,1,31.7
```

applies a mass flow rate of 31.7 to node 73. To have any effect, this node must be the midside node of a network element.

Example files: achteld.

7.4.3 Submodel

Submodel conditions can be defined between a *STEP card and an *END STEP card only.

First line:

- *BOUNDARY,SUBMODEL
- use the STEP parameter to specify the step in the global model

Following line:

- Node number or node set label
- First degree of freedom to be interpolated from the global model
- Last degree of freedom to be interpolated from the global model

Repeat this line if needed.

Example:

```
*BOUNDARY,SUBMODEL
73,1,3
```

specifies that all displacements in node 73 should be obtained by interpolation from the global model.

Example files: .

7.5 *BOUNDARYF

Keyword type: step

This option is used to prescribe boundary conditions for 3D-fluids calculations. This includes static temperature, velocity and static pressure.

The following degrees of freedom are being used:

- 1: velocity in the local x-direction
- 2: velocity in the local y-direction
- 3: velocity in the local z-direction
- 8: static pressure
- 11: static temperature

If no *TRANSFORM card applied to the node at stake, the local directions coincide with the global ones.

Optional parameters are AMPLITUDE, TIME DELAY, and USER. Their meaning is the same as for the *BOUNDARY card.

The main differences with the *BOUNDARY card are:

- the *BOUNDARYF card can only be used within a step
- for fluids the boundary conditions are applied to element faces and not to nodes.

Thus, the cards run like:

First line:

- *BOUNDARYF
- Enter any needed parameters and their value.

Following line:

- Element number or element set label
- Local face number of the element
- First degree of freedom constrained
- Last degree of freedom constrained. This field may be left blank if only one degree of freedom is constrained.
- Actual magnitude of the prescribed displacement (default is zero)

Repeat this line if needed. For the local face numbering the reader is referred to the *DLOAD card.

```
Example:

*BOUNDARYF
22,S3,2,2,.1
```

assigns to degree of freedom two of local face 3 of element 22 the value 0.1. If no transformation applies this degree of freedom corresponds to the velocity in global y-direction.

7.6 *BUCKLE

Keyword type: step

This procedure is used to determine the buckling load of a structure. The load active in the last non-perturbative *STATIC step, if any, will be taken as preload if the perturbation parameter is specified on the *STEP card. All loads previous to a perturbation step are removed at the start of the step; only the load specified within the buckling step is scaled till buckling occurs. Right now, only the stress stiffness due to the buckling load is taken into account and not the large deformation stiffness it may cause.

Buckling leads to an eigenvalue problem whose lowest eigenvalue is the scalar the load in the buckling step has to be multiplied with to get the buckling load. Thus, generally only the lowest eigenvalue is needed. This value is also called the buckling factor and it is always stored in the .dat file.

SOLVER is the only parameter. It specifies which solver is used to determine the stress stiffness due to the buckling load and to perform a decomposition of the linear equation system. This decomposition is done only once. It is repeatedly used in the iterative procedure determining the eigenvalues (the buckling factor). The following solvers can be selected:

- the SGI solver
- PARDISO
- SPOOLES [3, 4].
- TAUCS

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, no eigenvalue analysis can be performed.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU

decomposition, however, I was not able to run either of them so far. PARDISO is the Intel proprietary solver.

First line:

- *BUCKLE

Second line:

- Number of buckling factors desired (usually 1).
- Accuracy desired (default: 0.01).
- # Lanczos vectors calculated in each iteration (default: 4 * #eigenvalues).
- Maximum # of iterations (default: 1000).

It is rarely needed to change the defaults.

The eigenvalues are automatically stored in file jobname.dat.

```
Example:

*BUCKLE
2
```

calculates the lowest two buckling modes and the corresponding buckling factors. For the accuracy, the number of Lanczos vectors and the number of iterations the defaults are taken.

Example files: beam8b,beamb.

7.7 *CFLUX

Keyword type: step

This option allows concentrated heat fluxes to be applied to any node in the model which is not fixed by a single or multiple point constraint. Optional parameters are OP, AMPLITUDE, TIME DELAY, USER and ADD. OP can take the value NEW or MOD. OP=MOD is default and implies that the concentrated fluxes applied to different nodes in previous steps are kept. Specifying a flux in a node for which a flux was defined in a previous step replaces this value. A flux specified in a node for which a flux was already defined within the same step is added to this value. OP=NEW implies that all concentrated fluxes applied in previous steps are removed. If multiple *CFLUX cards are present in a step this parameter takes effect for the first *CFLUX card only.

The AMPLITUDE parameter allows for the specification of an amplitude by which the flux values are scaled (mainly used for nonlinear static and dynamic calculations). Thus, in that case the values entered on the *CFLUX card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference

value is replaced by the actual value at that time. In subsequent steps this value is kept constant unless it is explicitly redefined or the amplitude is defined using TIME=TOTAL TIME in which case the amplitude keeps its validity.

The TIME DELAY parameter modifies the AMPLITUDE parameter. As such, TIME DELAY must be preceded by an AMPLITUDE name. TIME DELAY is a time shift by which the AMPLITUDE definition it refers to is moved in positive time direction. For instance, a TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The TIME DELAY parameter must only appear once on one and the same keyword card.

If the USER parameter is selected the concentrated flux values are determined by calling the user subroutine cflux.f, which must be provided by the user. This applies to all nodes listed beneath the *CFLUX keyword. Any flux values specified following the temperature degree of freedom are not taken into account. If the USER parameter is selected, the AMPLITUDE parameter has no effect and should not be used.

Finally, the ADD parameter allows the user to specify that the flux should be added to previously defined fluxes in the same node, irrespective whether these fluxes were defined in the present step or in a previous step.

The use of the *CFLUX card makes sense for heat transfer calculations or coupled thermo-mechanical calculations only. Heat fluxes are applied to degree of freedom 11.

First line:

- *CFLUX
- Enter any needed parameters and their value.

Following line:

- Node number or node set label.
- Degree of freedom (11).
- Magnitude of the flux

Repeat this line if needed.

`Example:`

```
*CFLUX,OP=NEW,AMPLITUDE=A1
10,11,15.
```

removes all previous concentrated heat fluxes and applies a flux with magnitude 15. and amplitude A1 for degree of freedom 11 (this is the temperature degree of freedom) of node 10.

Example files: oneel20cf.

7.8 *CHANGE FRICTION

Keyword type: step

With this option one can redefine the contact friction value within a step. There is one required parameter INTERACTION, denoting the name of the *SURFACE INTERACTION the friction of which one would like to change. This card must be followed by a *FRICTION card to become effective.

First and only line:

- *CHANGE FRICTION
- enter the required parameter INTERACTION and its parameter.

Example:

```
*CHANGE FRICTION,INTERACTION=IN1
```

indicates that the friction value of surface interaction IN1 is to be changed to the value underneath the following *FRICTION card.

Example files: friction2

7.9 *CHANGE MATERIAL

Keyword type: step

With this option one can redefine material properties within a step. There is one required parameter NAME, denoting the name of the *MATERIAL. Right now, only plastic data of an elastically isotropic material with explicitly defined isotropic or kinematic hardening data can be changed. This card must be followed by a *CHANGE PLASTIC card to have any effect.

First and only line:

- *CHANGE MATERIAL
- enter the required parameter NAME and its parameter.

Example:

```
*CHANGE MATERIAL,NAME=PL
```

indicates that the plastic data of material PL are to be changed to the values underneath the following *CHANGE PLASTIC card.

Example files: beampiso2

7.10 *CHANGE PLASTIC

Keyword type: step

With this option one can redefine plastic data of an elastically isotropic material with explicitly defined isotropic or kinematic hardening data within a step. Combined hardening or user-defined hardening data are not allowed.

There is one optional parameter HARDENING. Default is HARDENING=ISOTROPIC, the only other value is HARDENING=KINEMATIC for kinematic hardening. All constants may be temperature dependent.

For the selection of plastic output variables the reader is referred to Section 6.8.6.

First line:

- *CHANGE PLASTIC
- Enter the HARDENING parameter and its value, if needed

Following sets of lines define the isotropic hardening curve for HARDENING=ISOTROPIC and the kinematic hardening curve for HARDENING=KINEMATIC: First line in the first set:

- Von Mises stress.
- Equivalent plastic strain.
- Temperature.

Use as many lines in the first set as needed to define the complete hardening curve for this temperature.

Use as many sets as needed to define complete temperature dependence. Notice that it is not allowed to use more plastic strain data points or temperature data points than the amount used for the first definition of the plastic behavior for this material (in the *PLASTIC card.

The raison d'être for this card is its ability to switch from purely plastic behavior to creep behavior and vice-versa. The viscoplastic for isotropic materials in CalculiX is an overstress model, i.e. creep only occurs above the yield stress. For a lot of materials this is not realistic. It is observed in blades and vanes that at high temperatures creep occurs at stresses well below the yield stress. By using the *CHANGE PLASTIC card the yield stress can be lowered to zero in a creep (*VISCO) step following a inviscid (*STATIC) plastic deformation step.

Example:

```
*CHANGE PLASTIC
0.,0.
0.,1.e10
```

defines a material with yield stress zero.

Example files: beampiso2

7.11 *CHANGE SURFACE BEHAVIOR

Keyword type: step

With this option one can redefine the contact surface behavior within a step. There is one required parameter INTERACTION, denoting the name of the *SURFACE INTERACTION the surface behavior of which one would like to change. This card must be followed by a *SURFACE BEHAVIOR card to become effective.

First and only line:

- *CHANGE SURFACE BEHAVIOR
- enter the required parameter INTERACTION and its parameter.

Example:

```
*CHANGE SURFACE BEHAVIOR,INTERACTION=IN1
```

indicates that the surface behavior value of surface interaction IN1 is to be changed to the value underneath the following *SURFACE BEHAVIOR card.

Example files: changesurfbeh

7.12 *CHANGE SOLID SECTION

Keyword type: step

This option is used to change material properties within a step for 3D, plane stress, plane strain or axisymmetric element sets. The parameters ELSET and MATERIAL are required, the parameter ORIENTATION is optional. The parameter ELSET defines the element set to which the material specified by the parameter MATERIAL applies. The parameter ORIENTATION allows to assign local axes to the element set. If activated, the material properties are applied to the local axis. This is only relevant for non isotropic material behavior.

It is not allowed to change the thickness, which is important for plane stress and plane strain elements. This is because these elements are expanded in three dimensional elements within the first step. So no second line is allowed.

Changing material properties may be used to activate or deactivate elements by assigning properties close to those of air to one material and the real properties to another material and switching between these.

First line:

- *CHANGE SOLID SECTION
- Enter any needed parameters.

Example:

```
*CHANGE SOLID SECTION,MATERIAL=EL,ELSET=Eall,ORIENTATION=OR1
```

reassigns material EL with orientation OR1 to all elements in (element) set Eall.

Example files: changesolidsection.

7.13 *CLEARANCE

Keyword type: model definition

With this option a clearance can be defined between the slave and master surface of a contact pair. It only applies to face-to-face contact. If this option is active, the actual clearance or overlapping based on the distance between the integration point on the slave surface and its orthogonal projection on the master surface is overwritten by the value specified here. There are three required parameters: MASTER, SLAVE and VALUE. With MASTER one specifies the master surface, with SLAVE the slave surface and with VALUE the value of the clearance. Only one value per contact pair is allowed.

First and only line:

- *CLEARANCE
- enter the required parameters and their values.

Example:

```
*CLEARANCE,MASTER=SURF1,SLAVE=SURF2,VALUE=0.1
```

indicates that the clearance between master surface SURF1 and slave surface SURF2 should be 0.1 length units. SURF1 and SURF2 must be used on one and the same *CONTACT PAIR card.

Example files:

7.14 *CLOAD

Keyword type: step

This option allows concentrated forces to be applied to any node in the model which is not fixed by a single or multiple point constraint. Optional parameters are OP, AMPLITUDE, TIME DELAY, USER, LOAD CASE, SECTOR, SUBMODEL and STEP. OP can take the value NEW or MOD. OP=MOD is default and implies that the concentrated loads applied to different nodes in previous steps are kept. Specifying a force in a node for which a force was defined in a previous step replaces this value. A force specified in a node and direction for

which a force was already defined within the same step is added to this value. OP=NEW implies that all concentrated loads applied in previous steps are removed. If multiple *CLOAD cards are present in a step this parameter takes effect for the first *CLOAD card only.

The AMPLITUDE parameter allows for the specification of an amplitude by which the force values are scaled (mainly used for nonlinear static and dynamic calculations). Thus, in that case the values entered on the *CLOAD card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference value is replaced by the actual value at that time. In subsequent steps this value is kept constant unless it is explicitly redefined or the amplitude is defined using TIME=TOTAL TIME in which case the amplitude keeps its validity.

The AMPLITUDE parameter applies to all loads specified by the same *CLOAD card. This means that, by using several *CLOAD cards, different amplitudes can be applied to the forces in different coordinate directions in one and the same node. An important exception to this rule are nodes in which a transformation applies (by using the *TRANSFORM card): an amplitude defined for such a node applies to ALL coordinate directions. If several are defined, the last one applies.

The TIME DELAY parameter modifies the AMPLITUDE parameter. As such, TIME DELAY must be preceded by an AMPLITUDE name. TIME DELAY is a time shift by which the AMPLITUDE definition it refers to is moved in positive time direction. For instance, a TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The TIME DELAY parameter must only appear once on one and the same keyword card.

If the USER parameter is selected the concentrated load values are determined by calling the user subroutine cload.f, which must be provided by the user. This applies to all nodes listed beneath the *CLOAD keyword. Any load values specified following the degree of freedom are not taken into account. If the USER parameter is selected, the AMPLITUDE parameter has no effect and should not be used.

The LOAD CASE parameter is only active in *STEADY STATE DYNAMICS calculations. LOAD CASE = 1 means that the loading is real or in-phase. LOAD CASE = 2 indicates that the load is imaginary or equivalently phase-shifted by 90°. Default is LOAD CASE = 1.

The SECTOR parameter can only be used in *MODAL DYNAMIC and *STEADY STATE DYNAMICS calculations with cyclic symmetry. The datum sector (the sector which is modeled) is sector 1. The other sectors are numbered in increasing order in the rotational direction going from the slave surface to the master surface as specified by the *TIE card. Consequently, the SECTOR parameters allows to apply a point load to any node in any sector. However, the only coordinate systems allowed in a node in which a force is applied in a sector different from the datum sector are restricted to the global carthesian system and a local cylindrical system. If the global coordinate system applies, the force defined by the user (in the global system) is simply copied to the appropriate sector without changing its direction. The user must make sure

the direction of the force is the one needed in the destination sector. If a local cylindrical system applies, this system must be identical with the one defined underneath the *CYCLIC SYMMETRY MODEL card. In that case, the force defined in the datum sector is rotated towards the destination sector, i.e. the radial, circumferential and axial part of the force is kept.

Finally, the SUBMODEL parameter specifies that the forces in the specified degrees of freedom of the nodes listed underneath will be obtained by interpolation from a global model. To this end these nodes have to be part of a *SUBMODEL,TYPE=NODE card. On the latter card the result file (frd file) of the global model is defined. The use of the SUBMODEL parameter requires the STEP parameter, specifying the step in the global model which will be used for the interpolation. Notice that the forces interpolated from the global model are not transformed, no matter what coordinate system is applied to the nodes in the submodel. Consequently, if the forces of the global model are stored in a local coordinate system, this local system also applies to the submodel nodes in which these forces are interpolated. One could say that the submodel nodes in which the forces of the global model are interpolated, inherit the coordinate system in which the forces of the global model were stored.

First line:

- *CLOAD
- Enter any needed parameters and their value.

Following line:

- Node number or node set label.
- Degree of freedom.
- Magnitude of the load

Repeat this line if needed.

```
Example:

*CLOAD,OP=NEW,AMPLITUDE=A1,TIME DELAY=20.
1000,3,10.3
```

removes all previous point load forces and applies a force with magnitude 10.3 and amplitude A1 (shifted in positive time direction by 20 time units) for degree of freedom three (global if no transformation was defined for node 1000, else local) of node 1000.

Example files: achtelp, beamdelay.

7.15 *COMPLEX FREQUENCY

Keyword type: step

This procedure card is used to determine frequencies taking into account Coriolis forces (cf. Section 6.9.3). It must be preceded by a *FREQUENCY step in which the eigenvalues and eigenmodes are calculated without Coriolis (do not forget to use the option STORAGE=YES in the frequency step, ensuring that the eigenmodes and eigenvalues are stored in a .eig file). The frequency step does not have to be in the same input deck. There is one required parameter CORIOLIS.

Finally, the number of eigenfrequencies requested should not exceed the corresponding number in the frequency step.

First line:

- *COMPLEX FREQUENCY
- use the required parameter CORIOLIS

Second line:

- Number of eigenfrequencies desired.

Example:

```
*COMPLEX FREQUENCY,CORIOLIS
10
```

requests the calculation of the 10 lowest eigenfrequencies and corresponding eigenmodes.

Example files: rotor.

7.16 *CONDUCTIVITY

Keyword type: model definition, material

This option is used to define the conductivity coefficients of a material. There is one optional parameter TYPE. Default is TYPE=ISO, other values are TYPE=ORTHO for orthotropic materials and TYPE=ANISO for anisotropic materials. All constants may be temperature dependent. The unit of the conductivity coefficients is energy per unit of time per unit of length per unit of temperature.

First line:

- *CONDUCTIVITY
- Enter the TYPE parameter and its values, if needed

Following line for TYPE=ISO:

- κ.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Following line for TYPE=ORTHO:

- κ_{11}.
- κ_{22}.
- κ_{33}.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Following line for TYPE=ANISO:

- κ_{11}.
- κ_{22}.
- κ_{33}.
- κ_{12}.
- κ_{13}.
- κ_{23}.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

`Example:`

```
*CONDUCTIVITY
50.,373.
100.,573.
```

tells you that the conductivity coefficient in a body made of this material is 50 at $T = 373$ and 100 at $T = 573$. Below $T = 373$ its value is set to 50, above $T = 573$ it is set to 100 and in between linear interpolation is applied.

Example files: beamhtbo, oneel20fi.

7.17 *CONTACT DAMPING

Keyword type: model definition

With this option a damping constant can be defined for contact elements. It is one of the optional cards one can use within a *SURFACE INTERACTION definition.

The contact damping is applied in normal direction to the master surface of the contact pair. The resulting damping force is the product of the damping coefficient with the local normal velocity difference between the master and slave surface. With the optional parameter TANGENT FRACTION the user can define what fraction of the damping coefficient should be used in tangential direction, default is zero. For a nonzero tangential damping a tangential force results from the product of the tangential damping constant multiplied with the local tangential velocity difference vector.

First line:

- *CONTACT DAMPING
- enter the TANGENT FRACTION parameter if needed

Second line:

- Damping constant.

No temperature dependence is allowed

Example:

```
*SURFACE INTERACTION,NAME=SI1
*SURFACE BEHAVIOR,PRESSURE-OVERCLOSURE=LINEAR
1.e7
*CONTACT DAMPING
1.e-4
```

defines a contact damping with value 10^{-4} for all contact pairs using the surface interaction SI1.

Example files: contdamp1, contdamp2.

7.18 *CONTACT FILE

Keyword type: step

This option is used to print selected nodal contact variables in file jobname.frd for subsequent viewing by CalculiX GraphiX. The following variables can be selected (the label is square brackets [] is the one used in the .frd file; for frequency calculations with cyclic symmetry both a real and an imaginary part may be stored, in all other cases only the real part is stored):

- CDIS [CONTACT(real), CONTACTI(imaginary)]: Relative contact displacements (for node-to-face contact in frequency calculations with cyclic symmetry only for the base sector)
- CSTR [CONTACT(real), CONTACTI(imaginary)]: Contact stresses (for node-to-face contact in frequency calculations with cyclic symmetry only for the base sector)
- CELS [CELS]: Contact energy
- PCON [PCONTAC; submenu: O=opening, SL=slip, P=pressure, SH=shear stress]: Magnitude and phase of the relative contact displacements and contact stresses in a frequency calculation with cyclic symmetry. PCON can only be requested for face-to-face penalty contact.

Since contact is modeled by nonlinear springs the contact energy corresponds to the spring energy. All variables are stored at the slave nodes.

The relative contact displacements constitute a vector with three components. The first component is the clearance, i.e. the distance between the slave node and the master surface. Only negative values are stored; they correspond to a penetration of the slave node into the master surface. Positive values (i.e. a proper clearance) are set to zero. The second and third component represent the projection of the relative displacement between the two contact surfaces onto the master surface. To this end two local tangential unit vectors are defined on the master surface; the first is the normalized projection of a vector along the global x-axis on the master surface. If the global x-axis is nearly orthogonal to the master surface, the projection of a vector along the global z-axis is taken. The second is the vector product of a vector locally normal to the master surface with the first tangential unit vector. Now, the components of the projection of the relative displacement between the two contact surfaces onto the master surface with respect to the first and the second unit tangential vector are the second and third component of CDIS, respectively. They are only calculated if a friction coefficient has been defined underneath *FRICTION.

In the same way the contact stresses constitute a vector, the first component of which is the contact pressure, while the second and third component are the components of the shear stress vector exerted by the slave surface on the master surface with respect to the first and second unit tangential vector, respectively.

The selected variables are stored for the complete model, but are only nonzero in the slave nodes of contact definitions.

The first occurrence of a *CONTACT FILE keyword card within a step wipes out all previous nodal contact variable selections for file output. If no *CONTACT FILE card is used within a step the selections of the previous step apply. If there is no previous step, no nodal contact variables will be stored.

There are two optional parameters: FREQUENCY and TIME POINTS. They are mutually exclusive.

FREQUENCY applies to nonlinear calculations where a step can consist of several increments. Default is FREQUENCY=1, which indicates that the

results of all increments will be stored. FREQUENCY=N with N an integer indicates that the results of every Nth increment will be stored. The final results of a step are always stored. If you only want the final results, choose N very big. The value of N applies to *OUTPUT,*ELEMENT OUTPUT, *EL FILE, *ELPRINT, *NODE OUTPUT, *NODE FILE, *NODE PRINT, *FACE PRINT, *CONTACT OUTPUT, *CONTACT FILE and *CONTACT PRINT. If the FREQUENCY parameter is used for more than one of these keywords with conflicting values of N, the last value applies to all. A frequency parameter stays active across several steps until it is overwritten by another FREQUENCY value or the TIME POINTS parameter.

With the parameter TIME POINTS a time point sequence can be referenced, defined by a *TIME POINTS keyword. In that case, output will be provided for all time points of the sequence within the step and additionally at the end of the step. No other output will be stored and the FREQUENCY parameter is not taken into account. Within a step only one time point sequence can be active. If more than one is specified, the last one defined on any of the keyword cards *EL FILE, *ELPRINT, *NODE FILE, *NODE PRINT, *FACE PRINT, *CONTACT FILE and *CONTACT PRINT will be active. The TIME POINTS option should not be used together with the DIRECT option on the procedure card. The TIME POINTS parameters stays active across several steps until it is replaced by another TIME POINTS value or the FREQUENCY parameter.

Notice that CDIS and CSTR results are stored together, i.e. specifying CDIS will automatically store CSTR too and vice versa.

First line:

- *CONTACT FILE
- Enter any needed parameters and their values.

Second line:

- Identifying keys for the variables to be printed, separated by commas.

Example:

```
*CONTACT FILE,TIME POINTS=T1
CDIS,CSTR
```

requests the storage of the relative contact displacements and contact stresses in the .frd file for all time points defined by the T1 time points sequence.

Example files: cubef2f2.

7.19 *CONTACT OUTPUT

Keyword type: step

This option is used to print selected nodal contact variables in file jobname.frd for subsequent viewing by CalculiX GraphiX. It is provided for compatibility reasons with ABAQUS. The options and its use are identical with the *CONTACT FILE keyword.

Example:

```
*CONTACT OUTPUT,TIME POINTS=T1
CDIS,CSTR
```

requests the storage of the relative contact displacements and contact stresses in the .frd file for all time points defined by the T1 time points sequence.

Example files: .

7.20 *CONTACT PAIR

Keyword type: model definition

This option is used to express that two surfaces can make contact. There is one required parameter: INTERACTION, and three optional parameters: TYPE, SMALL SLIDING and ADJUST. The dependent surface is called the slave surface, the independent surface is the master surface. Surfaces are defined using the *SURFACE keyword card. The dependent surface can be defined as a nodal surface (option TYPE=NODE on the *SURFACE keyword) or as an element face surface (default for the *SURFACE card), whereas the independent surface has to be defined as an element face surface. If you are using quadratic elements, or if you select face-to-face contact, however, the slave surface has to be defined based on element faces and not on nodes.

The INTERACTION parameter takes the name of the surface interaction (keyword *SURFACE INTERACTION) which applies to the contact pair. The surface interaction defines the nature of the contact (hard versus soft contact..)

The TYPE parameter can take the value NODE TO SURFACE or SURFACE TO SURFACE. NODE TO SURFACE triggers node-to-face penalty contact, SURFACE TO SURFACE face-to-face penalty contact. Default as of version 2.8p2 ist face-to-face penalty contact.

The SMALL SLIDING parameter only applies to node-to-face penalty contact. If it is not active, the contact is large sliding. This means that the pairing between the nodes belonging to the dependent surface and faces of the independent surface is performed anew in every iteration. If the SMALL SLIDING parameter is active, the pairing is done once at the start of every increment and kept during the complete increment. SMALL SLIDING usually converges better than LARGE SLIDING, since changes in the pairing can deteriorate the convergence rate.

The ADJUST parameter allows the user to move selected slave nodes at the start of the calculation (i.e. at the start of the first step) such that they make contact with the master surface. This is a change of coordinates, i.e. the geometry of the structure at the start of the calculation is changed. This can be helpful if due to inaccuracies in the modeling a slave node which should lie on the master surface at the start of the calculation actually does not. Especially in static calculations this can lead to a failure to detect contact in the first increment and large displacements (i.e. acceleration due to a failure to establish equilibrium). These large displacements may jeopardize convergence in any subsequent iteration. The ADJUST parameter can be used with a node set as argument or with a nonnegative real number. If a node set is selected, all nodes in the set are adjusted at the start of the calculation. If a real number is specified, all nodes for which the clearance is smaller or equal to this number are adjusted. Penetration is interpreted as a negative clearance and consequently all penetrating nodes are always adjusted, no matter how small the adjustment size (which must be nonnegative). Notice that large adjustments can lead to deteriorated element quality. The adjustments are done along a vector through the slave node and locally orthogonal to the master surface.

First line:

- *CONTACT PAIR
- enter the required parameter INTERACTION and any optional parameters.

Following line:

- Name of the slave surface (can be nodal or element face based).
- Name of the master surface (must be based on element faces).

Example:

```
*CONTACT PAIR,INTERACTION=IN1,ADJUST=0.01
dep,ind
```

defines a contact pair consisting of the surface dep as dependent surface and the element face surface ind as independent surface. The name of the surface interaction is IN1. All slave nodes for which the clearance is smaller than or equal to 0.01 will be moved onto the master surface.

Example files: contact1, contact2.

7.21 *CONTACT PRINT

Keyword type: step

This option is used to print selected contact nodal variables in file jobname.dat. The following variables can be selected:

- Relative contact displacements (key=CDIS)
- Contact stresses (key=CSTR)
- Contact spring energy (key=CELS)
- Number of contact elements (key=CNUM)

Contact quantities are stored for all active slave nodes in the model for node-to-face penalty contact and for all active integration points in the slave face for face-to-face penalty contact. The relative contact displacements and the stresses consist of one component normal to the master surface and two components tangential to it. Positive values of the normal components represent the normal material overlap and the pressure, respectively. The energy is a scalar quantity.

There are three parameters, FREQUENCY, TIME POINTS and TOTALS. FREQUENCY and TIME POINTS are mutually exclusive.

The parameter FREQUENCY is optional, and applies to nonlinear calculations where a step can consist of several increments. Default is FREQUENCY=1, which indicates that the results of all increments will be stored. FREQUENCY=N with N an integer indicates that the results of every Nth increment will be stored. The final results of a step are always stored. If you only want the final results, choose N very big. The value of N applies to *OUTPUT,*ELEMENT OUTPUT, *EL FILE, *ELPRINT, *NODE OUTPUT, *NODE FILE, *NODE PRINT, *FACE PRINT,*CONTACT OUTPUT, *CONTACT FILE and *CONTACT PRINT. If the FREQUENCY parameter is used for more than one of these keywords with conflicting values of N, the last value applies to all. A frequency parameter stays active across several steps until it is overwritten by another FREQUENCY value or the TIME POINTS parameter.

With the parameter TIME POINTS a time point sequence can be referenced, defined by a *TIME POINTS keyword. In that case, output will be provided for all time points of the sequence within the step and additionally at the end of the step. No other output will be stored and the FREQUENCY parameter is not taken into account. Within a step only one time point sequence can be active. If more than one is specified, the last one defined on any of the keyword cards *NODE FILE, *EL FILE, *NODE PRINT, *EL PRINT or *FACE PRINT will be active. The TIME POINTS option should not be used together with the DIRECT option on the procedure card. The TIME POINTS parameters stays active across several steps until it is replaced by another TIME POINTS value or the FREQUENCY parameter.

The first occurrence of an *CONTACT PRINT keyword card within a step wipes out all previous contact variable selections for print output. If no *CONTACT PRINT card is used within a step the selections of the previous step apply, if any.

The parameter TOTALS only applies to the energy. If TOTALS=YES the sum of the contact spring energy for all contact definitions is printed in addition to their value for each active slave node (node-to-face contact) or active slave face integration point (face-to-face contact) separately. If TOTALS=ONLY is

selected the sum is printed but the individual contributions are not. If TOTALS=NO (default) the individual contributions are printed, but their sum is not.

If the model contains axisymmetric elements the spring energy applies to a segment of 2°. So for the total spring energy this value has to be multiplied by 180.

First line:

- *CONTACT PRINT

Second line:

- Identifying keys for the variables to be printed, separated by commas.

Example:

```
*CONTACT PRINT
CDIS
```

requests the storage of the relative displacements in all slave nodes in the .dat file.

Example files: beampkin, beamrb.

7.22 *CONTROLS

Keyword type: step

This option is used to change the iteration control parameters. It should only be used by those users who know what they are doing and are expert in the field. There are two, mutually exclusive parameter: PARAMETERS and RESET. The RESET parameter resets the control parameters to their defaults. With the parameter PARAMETERS is used to change the defaults. It can take the value TIME INCREMENTATION, FIELD or LINE SEARCH. If the TIME INCREMENTATION value is selected, the number of iterations before certain actions are taken (e.g. the number of divergent iterations before the increment is reattempted) can be changed and effect of these actions (e.g. the increment size is divided by two). The FIELD parameter can be used to change the convergence criteria themselves.

Finally, LINE SEARCH can be used to change the line search parameters (only for face-to-face penalty contact). The line search parameter scales the correction to the solution calculated by the Newton-Raphson algorithm such that the residual force is orthogonal to the correction. This requires the solution of a nonlinear equation, and consequently an iterative procedure. In CalculiX this procedure is approximated by a linear connection between:

- the scalar product of the residual force from the last iteration with the solution correction in the present iteration (corresponds to a line search paramter of zero) and

- the scalar product of the residual force in the present iteration with the solution correction in the present iteration (corresponds to a line search parameter of one).

For details of the line seach algorithm the reader is referred to [78].
First line:

- *CONTROLS
- Enter the PARAMETERS parameter and its value, or the RESET parameter.

There are no subsequent lines if the parameter RESET is selected.
Following lines if PARAMETERS=TIME INCREMENTATION is selected:
Second line:

- I_0 iteration after which a check is made whether the residuals increase in two consecutive iterations (default: 4). If so, the increment is reattempted with D_f times its size.
- I_R iteration after which a logarithmic convergence check is performed in each iteration (default: 8). If more than I_C iterations are needed, the increment is reattempted with D_C its size.
- I_P iteration after which the residual tolerance R_p^α is used instead of R_n^α (default: 9).
- I_C maximum number of iterations allowed (default: 16).
- I_L number of iterations after which the size of the subsequent increment will be reduced (default: 10).
- I_G maximum number of iterations allowed in two consecutive increments for the size of the next increment to be increased (default: 4).
- I_S Currently not used.
- I_A Maximum number of cutbacks per increment (default: 5). A cutback is a reattempted increment.
- I_J Currently not used.
- I_T Currently not used.

Third line:

- D_f Cutback factor if the solution seems to diverge(default: 0.25).
- D_C Cutback factor if the logarithmic extrapolation predicts too many iterations (default: 0.5).
- D_B Cutback factor for the next increment if more than I_L iterations were needed in the current increment (default: 0.75).

- D_A Cutback factor if the temperature change in two subsequent increments exceeds DELTMX (default: 0.85).
- D_S Currently not used.
- D_H Currently not used.
- D_D Factor by which the next increment will be increased if less than I_G iterations are needed in two consecutive increments (default: 1.5).
- W_G Currently not used.

Following lines if PARAMETERS=FIELD is selected:
Second line:

- R_n^α Convergence criterion for the ratio of the largest residual to the average force (default: 0.005). The average force is defined as the average over all increments in the present step of the instantaneous force. The instantaneous force in an increment is defined as the mean of the absolute value of the nodal force components within all elements.
- C_n^α Convergence criterion for the ratio of the largest solution correction to the largest incremental solution value (default: 0.01).
- q_0^α Initial value at the start of a new step of the time average force (default: the time average force from the previous steps or 0.01 for the first step).
- q_u^α user-defined average force. If defined, the calculation of the average force is replaced by this value.
- R_p^α Alternative residual convergence criterion to be used after I_P iterations instead of R_n^α (default: 0.02).
- ϵ^α Criterion for zero flux relative to q^α (default: 10^{-5}).
- C_ϵ^α Convergence criterion for the ratio of the largest solution correction to the largest incremental solution value in case of zero flux (default: 10^{-3}).
- R_l^α Convergence criterion for the ratio of the largest residual to the average force for convergence in a single iteration (default: 10^{-8}).

Following lines if PARAMETERS=LINE SEARCH is selected:
Second line:

- not used.
- s_{max}^{ls} Maximum value of the line search parameter (default: 1.).
- s_{min}^{ls} Minimum value of the line search parameter (default: 0.25).
- not used.

- not used.

Example:

```
*CONTROLS,PARAMETERS=FIELD
1.e30,1.e30,0.01,,0.02,1.e-5,1.e-3,1.e-8
```

leads to convergence in just one iteration since nearly any residuals are accepted for convergence ($R_n^\alpha = 10^{30}$ and $C_n^\alpha = 10^{30}$.

Example files: beammrco.

7.23 *COUPLED TEMPERATURE-DISPLACEMENT

Keyword type: step

This procedure is used to perform a coupled thermomechanical analysis. A thermomechanical analysis is a nonlinear calculation in which the displacements and temperatures are simultaneously solved. In this way the reciprocal action of the temperature on the displacements and the displacements on the temperature can be taken into account. At the present state, the influence of the temperature on the displacements is calculated through the thermal expansion, the effect of the displacements on the temperature is limited to radiation effects. In addition, the influence of the network fluid pressure on the deformation of a structure and the influence of the structural deformation on the network fluid mass flow can be considered. Other heating effects, e.g. due to plasticity, or not yet taken into account. This card is also correct for CFD-calculations with heat transfer.

There are seven optional parameters: SOLVER, DIRECT, ALPHA, STEADY STATE, DELTMX, TIME RESET and TOTAL TIME AT START.

SOLVER determines the package used to solve the ensuing system of equations. The following solvers can be selected:

- the SGI solver
- PARDISO
- SPOOLES [3, 4].
- TAUCS
- the iterative solver by Rank and Ruecker [60], which is based on the algorithms by Schwarz [64].

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, the default is the iterative solver, which comes with the CalculiX package.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no

out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU decomposition, however, I was not able to run either of them so far. Next comes the iterative solver. If SOLVER=ITERATIVE SCALING is selected, the pre-conditioning is limited to a scaling of the diagonal terms, SOLVER=ITERATIVE CHOLESKY triggers Incomplete Cholesky pre-conditioning. Cholesky pre-conditioning leads to a better convergence and maybe to shorter execution times, however, it requires additional storage roughly corresponding to the non-zeros in the matrix. If you are short of memory, diagonal scaling might be your last resort. The iterative methods perform well for truly three-dimensional structures. For instance, calculations for a hemisphere were about nine times faster with the ITERATIVE SCALING solver, and three times faster with the ITERATIVE CHOLESKY solver than with SPOOLES. For two-dimensional structures such as plates or shells, the performance might break down drastically and convergence often requires the use of Cholesky preconditioning. SPOOLES (and any of the other direct solvers) performs well in most situations with emphasis on slender structures but requires much more storage than the iterative solver. PARDISO is the Intel proprietary solver.

The parameter DIRECT indicates that automatic incrementation should be switched off. The increments will have the fixed length specified by the user on the second line.

The parameter ALPHA takes an argument between -1/3 and 0. It controls the dissipation of the high frequency response: lower numbers lead to increased numerical damping ([53]). The default value is -0.05.

The parameter STEADY STATE indicates that only the steady state should be calculated. If this parameter is absent, the calculation is assumed to be time dependent and a transient analysis is performed. For a transient analysis the specific heat of the materials involved must be provided. In a steady state analysis any loading is applied using linear ramping, in a transient analysis step loading is applied.

The parameter DELTMX can be used to limit the temperature change in two subsequent increments. If the temperature change exceeds DELTMX the increment is restarted with a size equal to D_A times DELTMX divided by the temperature change. The default for D_A is 0.85, however, it can be changed by the *CONTROLS keyword. DELTMX is only active in transient calculations. Default value is 10^{30}.

The parameter TIME RESET can be used to force the total time at the end of the present step to coincide with the total time at the end of the previous step. If there is no previous step the targeted total time is zero. If this parameter is absent the total time at the end of the present step is the total time at the end of the previous step plus the time period of the present step (2nd parameter underneath the *COUPLED TEMPERATURE-DISPLACEMENT keyword). Consequently, if the time at the end of the previous step is 10. and the present time period is 1., the total time at the end of the present step is 11. If the

TIME RESET parameter is used, the total time at the beginning of the present step is 9. and at the end of the present step it will be 10. This is sometimes useful if transient coupled temperature-displacement calculations are preceded by a stationary heat transfer step to reach steady state conditions at the start of the transient coupled temperature-displacement calculations. Using the TIME RESET parameter in the stationary step (the first step in the calculation) will lead to a zero total time at the start of the subsequent instationary step.

Finally, the parameter TOTAL TIME AT START can be used to set the total time at the start of the step to a specific value.

First line:

- *COUPLED TEMPERATURE-DISPLACEMENT
- Enter any needed parameters and their values.
- Initial time increment. This value will be modified due to automatic incrementation, unless the parameter DIRECT was specified (default 1.).
- Time period of the step (default 1.).
- Minimum time increment allowed. Only active if DIRECT is not specified. Default is the initial time increment or 1.e-5 times the time period of the step, whichever is smaller.
- Maximum time increment allowed. Only active if DIRECT is not specified. Default is 1.e+30.
- Initial time increment for CFD applications (default 1.e-2)

Example:

```
*COUPLED TEMPERATURE-DISPLACEMENT
.1,1.
```

defines a thermomechanical step and selects the SPOOLES solver as linear equation solver in the step (default). The second line indicates that the initial time increment is .1 and the total step time is 1.

Example files: thermomech.

7.24 *CREEP

Keyword type: model definition, material

This option is used to define the creep properties of a viscoplastic material. There is one optional parameter LAW. Default is LAW=NORTON, the only other value is LAW=USER for a user-defined creep law. The Norton law satisfies:

$$\dot{\epsilon} = A\sigma^n t^m \tag{332}$$

where ϵ is the equivalent creep strain, σ is the true Von Mises stress an t is the total time. For LAW=USER the creep law must be defined in user subroutine creep.f.

All constants may be temperature dependent. The card should be preceded by a *ELASTIC card within the same material definition, defining the elastic properties of the material. If for LAW=NORTON the temperature data points under the *CREEP card are not the same as those under the *ELASTIC card, the creep data are interpolated at the *ELASTIC temperature data points. If a *PLASTIC card is defined within the same material definition, it should be placed after the *ELASTIC and before the *CREEP card. If no *PLASTIC card is found, a zero yield surface without any hardening is assumed.

If the elastic data is isotropic, the large strain viscoplastic theory treated in [68] and [69] is applied. If the elastic data is orthotropic, the infinitesimal strain model discussed in Section 6.8.11 is used. If a *PLASTIC card is used for an orthotropic material, the LAW=USER option is not available.

First line:

- *CREEP
- Enter the LAW parameter and its value, if needed

Following lines are only needed for LAW=NORTON (default): First line:

- A.
- n.
- m.
- Temperature.

Use as many lines as needed to define the complete temperature dependence.

`Example:`

```
*CREEP
1.E-10,5.,0.,100.
2.E-10,5.,0.,200.
```

defines a creep law with A=10^{-10}, n=5 and m=0 for T(temperature)=100. and A=$2 \cdot 10^{-10}$ and n=5 for T(temperature)=200.

Example files: beamcr.

7.25 *CYCLIC HARDENING

Keyword type: model definition,material

This option is used to define the isotropic hardening curves of an incrementally plastic material with combined hardening. All constants may be temperature dependent. The card should be preceded by an *ELASTIC card within the same material definition, defining the isotropic elastic properties of the material.

If the elastic data is isotropic, the large strain viscoplastic theory treated in [68] and [69] is applied. If the elastic data is orthotropic, the infinitesimal strain model discussed in Section 6.8.11 is used. Accordingly, for an elastically orthotropic material the hardening can be at most linear. Furthermore, if the temperature data points for the hardening curves do not correspond to the *ELASTIC temperature data points, they are interpolated at the latter points. Therefore, for an elastically isotropic material, it is advisable to define the hardening curves at the same temperatures as the elastic data.

Please note that, for each temperature, the (von Mises stress,equivalent plastic strain) data have to be entered in ascending order of the equivalent plastic strain.

First line:

- *CYCLIC HARDENING

Following sets of lines defines the isotropic hardening curve: First line in the first set:

- Von Mises stress.
- Equivalent plastic strain.
- Temperature.

Use as many lines in the first set as needed to define the complete hardening curve for this temperature.

Use as many sets as needed to define complete temperature dependence.

Example:

```
*CYCLIC HARDENING
800.,0.,100.
1000.,.1,100.
900.,0.,500.
1050.,.11,500.
```

defines two (stress,plastic strain) data points at T=100. and two data points at T=500. Notice that the temperature must be listed in ascending order. The same is true for the plastic strain within a temperature block.

Example files: beampik.

7.26 *CYCLIC SYMMETRY MODEL

Keyword type: model definition

This keyword is used to define the number of sectors and the axis of symmetry in a cyclic symmetric structure for use in a cyclic symmetry calculation. It must be preceded by two *SURFACE cards defining the nodes belonging to the left and right boundary of the sector and a *TIE card linking those surfaces. The axis of symmetry is defined by two points a and b, defined in global Cartesian coordinates.

There are five parameters, N, NGRAPH, TIE, ELSET and CHECK. The parameter N, specifying the number of sectors, is required, TIE is required if more than one cyclic symmetry tie is defined.

The parameter NGRAPH is optional and indicates for how many sectors the solutions should be stored in .frd format. Setting NGRAPH=N for N sectors stores the solution for the complete structure for subsequent plotting purposes. Default is NGRAPH=1.

The parameter TIE specifies the name of the tie constraint to which the cyclic symmetry model definition applies. It need not be specified if only one *TIE card has been defined.

The element set specified by ELSET specifies the elements to which the parameter NGRAPH should be applied. Default if only one *TIE card was used is the complete model.

The last parameter, CHECK, specifies whether CalculiX should compare the sector angle based on its geometry with its value based on N. If CHECK=NO is specified, the check is not performed, else it is. If the user wants to find eigenmodes with fractional nodal diameters, i.e. vibrations for which the phase shift is smaller than the sector angle, a value of N has to be specified which exceeds the number of sectors in the model. In that case the check should be turned off.

Several *CYCLIC SYMMETRY MODEL cards within one input deck defining several cyclic symmetries within one and the same model are allowed. This, however, always is an approximation, since several cyclic symmetries within one model cannot really exist. Good results are only feasible if the values of N for the different *CYCLIC SYMMETRY MODEL cards do not deviate substantially.

The *CYCLIC SYMMETRY MODEL card triggers the creation of cyclic symmetry multiple point constraints between the slave and master side. If the nodes do not match on a one-to-one basis a slave node is connected to a master face. To this end the master side is triangulated. The resulting triangulation is stored in file TriMasterCyclicSymmetryModel.frd and can be viewed with CalculiX GraphiX.

First line:

- *CYCLIC SYMMETRY MODEL
- Enter the required parameters N and TIE (the latter only if more than one cyclic symmetry tie is defined) and their value.

Second line:

- X-coordinate of point a.
- Y-coordinate of point a.
- Z-coordinate of point a.
- X-coordinate of point b.
- Y-coordinate of point b.
- Z-coordinate of point b.

`Example:`

```
*CYCLIC SYMMETRY MODEL, N=12, NGRAPH=3
0.,0.,0.,1.,0.,0.
```

defines a cyclic symmetric structure consisting of 30° sectors and axis of symmetry through the points (0.,0.,0.) and (1.,0.,0.). The solution will be stored for three connected sectors (120°).

Example files: segment, fullseg.

7.27 *DAMPING

Keyword type: model definition

This card is used to define Rayleigh damping for implicit dynamic calculations (*DYNAMIC). There are two required parameters: ALPHA and BETA.

Rayleigh damping is applied in a global way, i.e. the damping matrix $[C]$ is taken to be a linear combination of the stiffness matrix $[K]$ and the mass matrix $[M]$:

$$[C] = \alpha [M] + \beta [K] . \tag{333}$$

Right now, only one *DAMPING card can be used in the input deck. It applies to the whole model.

First line:

- *DAMPING
- Enter ALPHA and BETA and their values.

`Example:`

```
*DAMPING,ALPHA=5000.,BETA=2.e-3
```

indicates that a damping matrix is created by multiplying the mass matrix with 5000. and adding it to the stiffness matrix multiplied by $2 \cdot 10^{-4}$

Example files: beamimpdy1, beamimpdy2.

7.28 *DASHPOT

Keyword type: model definition

With this option the force-velocity relationship can be defined for dashpot elements. There is one required parameter ELSET. With this parameter the element set is referred to for which the dashpot behavior is defined. This element set should contain dashpot elements of type DASHPOTA only.

The dashpot constant can depend on frequency and temperature. Frequency dependence only makes sense for *STEADY STATE DYNAMICS calculations.

First line:

- *DASHPOT
- Enter the parameter ELSET and its value

Second line: enter a blank line

For each temperature a set of lines can be entered. First line in the first set:

- Dashpot constant.
- Frequency (only for steady state dynamics calculations, else blank).
- Temperature.

Use as many lines in the first set as needed to define the complete frequency dependence of the dashpot constant (if applicable) for this temperature. Use as many sets as needed to define complete temperature dependence.

Example:

```
*DASHPOT,ELSET=Eall
1.e-5
```

defines a dashpot constant with value 10^{-5} for all elements in element set Eall and all temperatures.

Example:

```
*DASHPOT,ELSET=Eall
1.e-5,1000.,273.
1.e-6,2000.,273.
1.e-4,,373.
```

defines a dashpot constant with value 10^{-5} at a frequency of 1000 and with value 10^{-6} at a frequency of 2000, both at a temperature of 273. At a temperature of 373 the dashpot constant is frequency independent and takes the value 10^{-4}. These constants apply to all dashpot elements in set Eall.

Example files: dashpot1, dashpot2, dashpot3.

7.29 *DEFORMATION PLASTICITY

Keyword type: model definition, material

This option defines the elasto-plastic behavior of a material by means of the generalized Ramberg-Osgood law. The one-dimensional model takes the form:

$$E\epsilon = \sigma + \alpha \left(\frac{|\sigma|}{\sigma_0} \right)^{n-1} \sigma \tag{334}$$

where ϵ is the logarithmic strain and σ the Cauchy stress. In the present implementation, the Eulerian strain is used, which is very similar to the logarithmic strain (about 1.3 % difference dat 20 % engineering strain). All coefficients may be temperature dependent.

First line:

- *DEFORMATION PLASTICITY

Following line:

- Young's modulus (E).
- Poisson's ratio (ν).
- Yield stress (σ_0)
- Exponent (n).
- Yield offset (α).
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Example:

```
*DEFORMATION PLASTICITY
210000.,.3,800.,12.,0.4
```

defines a Ramberg-Osgood law. No temperature dependence is introduced.

Example files: beampl.

7.30 *DENSITY

Keyword type: model definition, material

With this option the mass density of a material can be defined. The mass density is required for a frequency analysis (*FREQUENCY), for a dynamic analysis (*DYNAMIC or *HEAT TRANSFER) and for a static analysis with gravity loads (GRAV) or centrifugal loads (CENTRIF). The density can be temperature dependent.

First line:

- *DENSITY

Following line:

- Mass density.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Example:

```
*DENSITY
7.8E-9
```

defines a density with value 7.8×10^{-9} for all temperatures.

Example files: achtelc, segment1, segment2, beamf.

7.31 *DEPVAR

Keyword type: model definition, material

This keyword is used to define the number of internal state variables for a user-defined material. They are initialized to zero at the start of the calculation and can be used within a material user subroutine. There are no parameters. This card must be preceded by a *USER MATERIAL card.

First line:

- *DEPVAR

Second line:

- Number of internal state variables.

Example:

```
*DEPVAR
12
```

defines 12 internal state variables for the user-defined material at stake.

Example files: .

7.32 *DFLUX

Keyword type: step

This option allows the specification of distributed heat fluxes. These include surface flux (energy per unit of surface per unit of time) on element faces and volume flux in bodies (energy per unit of volume per unit of time).

In order to specify which face the flux is entering or leaving the faces are numbered. The numbering depends on the element type.

For hexahedral elements the faces are numbered as follows (numbers are node numbers):

- Face 1: 1-2-3-4
- Face 2: 5-8-7-6
- Face 3: 1-5-6-2
- Face 4: 2-6-7-3
- Face 5: 3-7-8-4
- Face 6: 4-8-5-1

for tetrahedral elements:

- Face 1: 1-2-3
- Face 2: 1-4-2
- Face 3: 2-4-3
- Face 4: 3-4-1

for wedge elements:

- Face 1: 1-2-3
- Face 2: 4-5-6
- Face 3: 1-2-5-4
- Face 4: 2-3-6-5
- Face 5: 3-1-4-6

for quadrilateral plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-4
- Face 4: 4-1

- Face N: in negative normal direction (only for plane stress)
- Face P: in positive normal direction (only for plane stress)

for triangular plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-1
- Face N: in negative normal direction (only for plane stress)
- Face P: in positive normal direction (only for plane stress)

for quadrilateral shell elements:

- Face NEG or 1: in negative normal direction
- Face POS or 2: in positive normal direction
- Face 3: 1-2
- Face 4: 2-3
- Face 5: 3-4
- Face 6: 4-1

for triangular shell elements:

- Face NEG or 1: in negative normal direction
- Face POS or 2: in positive normal direction
- Face 3: 1-2
- Face 4: 2-3
- Face 5: 3-1

The labels NEG and POS can only be used for uniform flux and are introduced for compatibility with ABAQUS. Notice that the labels 1 and 2 correspond to the brick face labels of the 3D expansion of the shell (Figure 61).

for beam elements:

- Face 1: in negative 1-direction
- Face 2: in positive 1-direction
- Face 3: in positive 2-direction
- Face 5: in negative 2-direction

The beam face numbers correspond to the brick face labels of the 3D expansion of the beam (Figure 66).

The surface flux is entered as a uniform flux with distributed flux type label Sx where x is the number of the face. For flux entering the body the magnitude of the flux is positive, for flux leaving the body it is negative. If the flux is nonuniform the label takes the form SxNUy and a user subroutine dflux.f must be provided specifying the value of the flux. The label can be up to 20 characters long. In particular, y can be used to distinguish different nonuniform flux patterns (maximum 16 characters).

For body generated flux (energy per unit of time per unit of volume) the distributed flux type label is BF for uniform flux and BFNUy for nonuniform flux. For nonuniform flux the user subroutine dflux must be provided. Here too, y can be used to distinguish different nonuniform body flux patters (maximum 16 characters).

Optional parameters are OP, AMPLITUDE and TIME DELAY. OP takes the value NEW or MOD. OP=MOD is default and implies that the surface fluxes on different faces in previous steps are kept. Specifying a distributed flux on a face for which such a flux was defined in a previous step replaces this value, if a flux was defined for the same face within the same step it is added. OP=NEW implies that all previous surface flux is removed. If multiple *DFLUX cards are present in a step this parameter takes effect for the first *DFLUX card only.

The AMPLITUDE parameter allows for the specification of an amplitude by which the flux values are scaled (mainly used for dynamic calculations). Thus, in that case the values entered on the *DFLUX card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference value is replaced by the actual value at that time. In subsequent steps this value is kept constant unless it is explicitly redefined or the amplitude is defined using TIME=TOTAL TIME in which case the amplitude keeps its validity. The AMPLITUDE parameter has no effect on nonuniform fluxes.

The TIME DELAY parameter modifies the AMPLITUDE parameter. As such, TIME DELAY must be preceded by an AMPLITUDE name. TIME DELAY is a time shift by which the AMPLITUDE definition it refers to is moved in positive time direction. For instance, a TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The TIME DELAY parameter must only appear once on one and the same keyword card.

First line:

- *DFLUX
- Enter any needed parameters and their value

Following line for surface flux:

- Element number or element set label.
- Distributed flux type label.

- Actual magnitude of the load (power per unit of surface).

Repeat this line if needed.

Following line for body flux:

- Element number or element set label.
- Distributed flux type label (BF or BFNU).
- Actual magnitude of the load (power per unit of volume).

Repeat this line if needed.

Example:

```
*DFLUX,AMPLITUDE=A1
20,S1,10.
```

assigns a flux entering the surface with magnitude 10 times the value of amplitude A1 to surface 1 of element 20.

Example:

```
*DFLUX
15,BF,10.
```

assigns a body flux with magnitude 10. to element 15.

Example files: oneel20df,beamhtbf.

7.33 *DISTRIBUTING COUPLING

Keyword type: model definition

This option is used to apply translational loading (force or displacement) on a set of nodes in a global sense (for rotations and/or moments the reader is referred to the mean rotation MPC, Section 8.7.1). There is one required parameter: ELSET. With the parameter ELSET an element set is referred to, which should contain exacty one element of type DCOUP3D. This type of element contains only one node, which is taken as the reference node of the distributing coupling. This node should not be used elsewhere in the model. In particular, it should not belong to any element. The coordinates of this node are immaterial. The distributing coupling forces or the distributing coupling displacements should be applied to the reference node with a *CLOAD card or a *BOUNDARY card, respectively.

Underneath the keyword card the user can enter the nodes on which the load is to be distributed, together with a weight. Internally, for each coordinate direction a multiple point constraint is generated between these nodes with the weights as coefficients. The last term in the equation is the reference node with as coefficient the negative of the sum of all weights.

First line:

- *DISTRIBUTING COUPLING
- Enter the ELSET parameter and its value

Following line:

- Node number or node set
- Weight

Repeat this line if needed.

Example:

```
*DISTRIBUTING COUPLING,ELSET=E1
3,1.
100,1.
51,1.
428,1.
*ELSET,ELSET=E1
823
*ELEMENT,TYPE=DCOUP3D
823,4000
```

defines a distributing coupling between the nodes 3, 100, 51 and 428, each with weight 1. The reference node is node 4000. A point force of 10 in direction 1 can be applied to this distributing coupling by the cards:

```
*CLOAD
4000,1,10.
```

while a displacement of 0.5 is obtained with

```
*BOUNDARY
4000,1,1,0.5
```

Example files: distcoup.

7.34 *DLOAD

Keyword type: step

This option allows the specification of distributed loads. These include constant pressure loading on element faces and mass loading (load per unit mass) either by gravity forces or by centrifugal forces.

For surface loading the faces of the elements are numbered as follows (for the node numbering of the elements see Section 3.1):

for hexahedral elements:

- face 1: 1-2-3-4
- face 2: 5-8-7-6
- face 3: 1-5-6-2
- face 4: 2-6-7-3
- face 5: 3-7-8-4
- face 6: 4-8-5-1

for tetrahedral elements:

- Face 1: 1-2-3
- Face 2: 1-4-2
- Face 3: 2-4-3
- Face 4: 3-4-1

for wedge elements:

- Face 1: 1-2-3
- Face 2: 4-5-6
- Face 3: 1-2-5-4
- Face 4: 2-3-6-5
- Face 5: 3-1-4-6

for quadrilateral plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-4
- Face 4: 4-1

for triangular plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-1

for beam elements:

- Face 1: pressure in 1-direction

- Face 2: pressure in 2-direction

For shell elements no face number is needed since there is only one kind of loading: pressure in the direction of the normal on the shell.

The surface loading is entered as a uniform pressure with distributed load type label Px where x is the number of the face. Thus, for pressure loading the magnitude of the load is positive, for tension loading it is negative. For nonuniform pressure the label takes the form PxNUy, and the user subroutine dload.f must be provided. The label can be up to 20 characters long. In particular, y can be used to distinguish different nonuniform loading patterns (maximum 16 characters). A typical example of a nonuniform loading is the hydrostatic pressure.

Another option is to assign the pressure of a fluid node to an element side. In that case the label takes the form PxNP, where NP stands for network pressure. The fluid node must be an corner node of a network element. Instead of a concrete pressure value the user must provide the fluid node number.

Optional parameters are OP, AMPLITUDE, TIME DELAY, LOAD CASE and SECTOR. OP takes the value NEW or MOD. OP=MOD is default. For surface loads it implies that the loads on different faces are kept from the previous step. Specifying a distributed load on a face for which such a load was defined in a previous step replaces this value, if a load was defined on the same face within the same step it is added. OP=NEW implies that all previous surface loading is removed. For mass loading the effect is similar. If multiple *DLOAD cards are present in a step this parameter takes effect for the first *DLOAD card only.

For centrifugal loading (label CENTRIF) the rotational speed square (ω^2) and two points on the rotation axis are required, for gravity loading with known gravity vector (label GRAV) the size and direction of the gravity vector are to be given. Whereas more than one centrifugal load for one and the same set is not allowed, several gravity loads can be defined, provided the direction of the load varies. If the gravity vector is not known it can be calculated based on the momentaneous mass distribution of the system (label NEWTON). This requires the value of the Newton gravity constant by means of a *PHYSICAL CONSTANTS card.

The limit of one centrifugal load per set does not apply to linear dynamic (*MODAL DYNAMIC) and steady state (*STEADY STATE DYNAMICS) calculations. Here, the limit is two. In this way a rotating eccentricity can be modeled. Prerequisite for the centrifugal loads to be interpreted as distinct is the choice of distinct rotation axes.

The AMPLITUDE parameter allows for the specification of an amplitude by which the force values are scaled (mainly used for dynamic calculations). Thus, in that case the values entered on the *DLOAD card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference value is replaced by the actual value at that time. In subsequent steps this value is kept constant unless it is explicitly redefined or the amplitude is defined using TIME=TOTAL

TIME in which case the amplitude keeps its validity. For nonuniform loading the AMPLITUDE parameter has no effect.

The TIME DELAY parameter modifies the AMPLITUDE parameter. As such, TIME DELAY must be preceded by an AMPLITUDE name. TIME DELAY is a time shift by which the AMPLITUDE definition it refers to is moved in positive time direction. For instance, a TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The TIME DELAY parameter must only appear once on one and the same keyword card.

The LOAD CASE parameter is only active in *STEADY STATE DYNAMICS calculations with harmonic loading. LOAD CASE = 1 means that the loading is real or in-phase. LOAD CASE = 2 indicates that the load is imaginary or equivalently phase-shifted by 90°. Default is LOAD CASE = 1.

The SECTOR parameter can only be used in *MODAL DYNAMIC and *STEADY STATE DYNAMICS calculations with cyclic symmetry. The datum sector (the sector which is modeled) is sector 1. The other sectors are numbered in increasing order in the rotational direction going from the slave surface to the master surface as specified by the *TIE card. Consequently, the SECTOR parameters allows to apply a distributed load to any element face in any sector.

First line:

- *DLOAD
- Enter any needed parameters and their value

Following line for surface loading:

- Element number or element set label.
- Distributed load type label.
- Actual magnitude of the load (for Px type labels) or fluid node number (for PxNU type labels)

Repeat this line if needed.

`Example:`

```
*DLOAD,AMPLITUDE=A1
Se1,P3,10.
```

assigns a pressure loading with magnitude 10. times the amplitude curve of amplitude A1 to face number three of all elements belonging to set Se1.

Example files: beamd.

Following line for centrifugal loading:

- Element number or element set label.
- CENTRIF
- rotational speed square (ω^2)
- Coordinate 1 of a point on the rotation axis
- Coordinate 2 of a point on the rotation axis
- Coordinate 3 of a point on the rotation axis
- Component 1 of the normalized direction of the rotation axis
- Component 2 of the normalized direction of the rotation axis
- Component 3 of the normalized direction of the rotation axis

Repeat this line if needed.

`Example:`

```
*DLOAD
Eall,CENTRIF,100000.,0.,0.,0.,1.,0.,0.
```

Example files: achtelc, disk2.
assigns centrifugal loading with $\omega^2 = 100000.$ about an axis through the point (0.,0.,0.) and with direction (1.,0.,0.) to all elements.

Following line for gravity loading with known gravity vector:

- Element number or element set label.
- GRAV
- Actual magnitude of the gravity vector.
- Coordinate 1 of the normalized gravity vector
- Coordinate 2 of the normalized gravity vector
- Coordinate 3 of the normalized gravity vector

Repeat this line if needed. Here "gravity" really stands for any acceleration vector.

`Example:`

```
*DLOAD
Eall,GRAV,9810.,0.,0.,-1.
```

assigns gravity loading in the negative z-direction with magnitude 9810. to all elements.

Example files: achtelg, cube2.

Following line for gravity loading based on the momentaneous mass distribution:

- Element number or element set label.
- NEWTON

Repeat this line if needed. Only elements loaded by a NEWTON type loading are taken into account for the gravity calculation.

```
Example:

*DLOAD
Eall,NEWTON
```

triggers the calculation of gravity forces due to all mass belonging to the element of element set Eall.

Example files: cubenewt.

7.35 *DSLOAD

Keyword type: step

This option allows for the specification of section stresses on the boundary of submodels, cf. the *SUBMODEL card. There are two required parameters: SUBMODEL and STEP. Underneath the *DSLOAD card faces are listed for which a section stress will be calculated by interpolation from the global model. To this end these faces have to be part of a *SUBMODEL card, TYPE=SURFACE. The latter card also lists the name of the global model results file. The STEP parameter specifies the step in the global model which will be used for the interpolation. The distributed load type label convention is the same as for the *DLOAD card.

First line:

- *DSLOAD
- Enter the parameter SUBMODEL (no argument) and STEP with its argument

Following line for surface loading:

- Element number or element set label.

- Distributed load type label.

Repeat this line if needed.

Example:

```
*DSLOAD,SUBMODEL,STEP=4
Se1,P3
```

specifies hat on face 3 of all elements belonging to set Se1 the section stress is to be determined by interpolation from step 4 in the global model.

Example files: .

7.36 *DYNAMIC

Keyword type: step

This procedure is used to calculate the response of a structure subject to dynamic loading using a direct integration procedure of the equations of motion. This card is also correct for transient incompressible flow calculations without heat transfer.

There are four optional parameters: DIRECT, ALPHA, EXPLICIT and SOLVER. The parameter DIRECT specifies that the user-defined initial time increment should not be changed. In case of no convergence with this increment size, the calculation stops with an error message. If this parameter is not set, the program will adapt the increment size depending on the rate of convergence. The parameter ALPHA takes an argument between -1/3 and 0. It controls the dissipation of the high frequency response: lower numbers lead to increased numerical damping ([53]). The default value is -0.05.

The parameter EXPLICIT can take the following values:

- 0: implicit structural computation, semi-implicit fluid computation
- 1: implicit structural computation, explicit fluid computation
- 2: explicit structural computation, semi-implicit fluid computation
- 3: explicit structural computation, explicit fluid computation

If the value is lacking, 3 is assumed. If the parameter is lacking altogether, a zero value is assumed.

The last parameter SOLVER determines the package used to solve the ensuing system of equations. The following solvers can be selected:

- the SGI solver
- PARDISO
- SPOOLES [3, 4].

- TAUCS
- the iterative solver by Rank and Ruecker [60], which is based on the algorithms by Schwarz [64].

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, the default is the iterative solver, which comes with the CalculiX package.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU decomposition, however, I was not able to run either of them so far. Next comes the iterative solver. If SOLVER=ITERATIVE SCALING is selected, the pre-conditioning is limited to a scaling of the diagonal terms, SOLVER=ITERATIVE CHOLESKY triggers Incomplete Cholesky pre-conditioning. Cholesky pre-conditioning leads to a better convergence and maybe to shorter execution times, however, it requires additional storage roughly corresponding to the non-zeros in the matrix. If you are short of memory, diagonal scaling might be your last resort. The iterative methods perform well for truly three-dimensional structures. For instance, calculations for a hemisphere were about nine times faster with the ITERATIVE SCALING solver, and three times faster with the ITERATIVE CHOLESKY solver than with SPOOLES. For two-dimensional structures such as plates or shells, the performance might break down drastically and convergence often requires the use of Cholesky preconditioning. SPOOLES (and any of the other direct solvers) performs well in most situations with emphasis on slender structures but requires much more storage than the iterative solver. PARDISO is the Intel proprietary solver.

In a dynamic step, loads are by default applied by their full strength at the start of the step. Other loading patterns can be defined by an *AMPLITUDE card.

First line:

- *DYNAMIC
- enter any parameters and their values, if needed.

Second line:

- Initial time increment. This value will be modified due to automatic incrementation, unless the parameter DIRECT was specified.
- Time period of the step.

- Minimum time increment allowed. Only active if DIRECT is not specified. Default is the initial time increment or 1.e-5 times the time period of the step, whichever is smaller.
- Maximum time increment allowed. Only active if DIRECT is not specified. Default is 1.e+30.
- Initial time increment for CFD applications (default 1.e-2)

Examples:

```
*DYNAMIC,DIRECT,EXPLICIT
1.E-7,1.E-5
```

defines an explicit dynamic procedure with fixed time increment 10^{-7} for a step of length 10^{-5}.

```
*DYNAMIC,ALPHA=-0.3,SOLVER=ITERATIVE CHOLESKY
1.E-7,1.E-5,1.E-9,1.E-6
```

defines an implicit dynamic procedure with variable increment size. The numerical damping was increased ($\alpha = -0.3$ instead of the default $\alpha = -0.05$, and the iterative solver with Cholesky pre-conditioning was selected. The starting increment has a size 10^{-7}, the subsequent increments should not have a size smaller than 10^{-9} or bigger than 10^{-6}. The step size is 10^{-5}.

Example files: beamnldy, beamnldye, beamnldyp, beamnldype.

7.37 *ELASTIC

Keyword type: model definition, material

This option is used to define the elastic properties of a material. There is one optional parameter TYPE. Default is TYPE=ISO, other values are TYPE=ORTHO and TYPE=ENGINEERING CONSTANTS for orthotropic materials and TYPE=ANISO for anisotropic materials. All constants may be temperature dependent. For orthotropic and fully anisotropic materials, the coefficients D_{IJKL} satisfy the equation:

$$S_{IJ} = D_{IJKL} E_{KL}, \quad I, J, K, L = 1..3 \tag{335}$$

where S_{IJ} is the second Piola-Kirchhoff stress and E_{KL} is the Lagrange deformation tensor (nine terms on the right hand side for each equation). For linear calculations, these reduce to the generic stress and strain tensors.

An isotropic material can be defined as an anisotropic material by defining $D_{1111} = D_{2222} = D_{3333} = \lambda + 2\mu$, $D_{1122} = D_{1133} = D_{2233} = \lambda$ and $D_{1212} = D_{1313} = D_{2323} = \mu$, where λ and μ are the Lamé constants [18].

First line:

- *ELASTIC
- Enter the TYPE parameter and its value, if needed

Following line for TYPE=ISO:

- Young's modulus.
- Poisson's ratio.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Following lines, in a pair, for TYPE=ORTHO: First line of pair:

- D_{1111}.
- D_{1122}.
- D_{2222}.
- D_{1133}.
- D_{2233}.
- D_{3333}.
- D_{1212}.
- D_{1313}.

Second line of pair:

- D_{2323}.
- Temperature.

Repeat this pair if needed to define complete temperature dependence.

Following lines, in a pair, for TYPE=ENGINEERING CONSTANTS: First line of pair:

- E_1.
- E_2.
- E_3.
- ν_{12}.
- ν_{13}.
- ν_{23}.

- G_{12}.
- G_{13}.

Second line of pair:

- G_{23}.
- Temperature.

Repeat this pair if needed to define complete temperature dependence.

Following lines, in sets of 3, for TYPE=ANISO: First line of set:

- D_{1111}.
- D_{1122}.
- D_{2222}.
- D_{1133}.
- D_{2233}.
- D_{3333}.
- D_{1112}.
- D_{2212}.

Second line of set:

- D_{3312}.
- D_{1212}.
- D_{1113}.
- D_{2213}.
- D_{3313}.
- D_{1213}.
- D_{1313}.
- D_{1123}.

Third line of set:

- D_{2223}.
- D_{3323}.
- D_{1223}.

- D_{1323}.
- D_{2323}.
- Temperature.

Repeat this set if needed to define complete temperature dependence.

Example:

```
*ELASTIC,TYPE=ORTHO
500000.,157200.,400000.,157200.,157200.,300000.,126200.,126200.,
126200.,294.
```

defines an orthotropic material for temperature T=294. Since the definition includes values for only one temperature, they are valid for all temperatures.

Example files: aniso, beampo1.

7.38 *ELECTRICAL CONDUCTIVITY

Keyword type: model definition, material

This option is used to define the electrical conductivity of a material. There are no parameters. The material is supposed to be isotropic. The constant may be temperature dependent. The unit of the electrical conductivity coefficient is one divided by the unit of resistivity (in SI-units: ohm) times the unit of length.

First line:

- *ELECTRICAL CONDUCTIVITY

Following line:

- σ.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Example:

```
*ELECTRICAL CONDUCTIVITY
5.96E7
```

tells you that the electrical conductivity coefficient is 5.96E7, independent of temperature (if SI-units are used this is the electrical conductivity of copper).

Example files: induction.

7.39 *ELECTROMAGNETICS

Keyword type: step

This procedure is used to perform a electromagnetic analysis. If transient, it may be combined with a heat analysis. In that case the calculation is nonlinear since the material properties depend on the solution, i.e. the temperature.

There are seven optional parameters: SOLVER, DIRECT, MAGNETOSTATICS, DELTMX, TIME RESET and TOTAL TIME AT START and NO HEAT TRANSFER.

SOLVER determines the package used to solve the ensuing system of equations. The following solvers can be selected:

- the SGI solver
- PARADISO
- SPOOLES [3, 4].
- TAUCS
- the iterative solver by Rank and Ruecker [60], which is based on the algorithms by Schwarz [64].

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, the default is the iterative solver, which comes with the CalculiX package.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU decomposition, however, I was not able to run either of them so far. Next comes the iterative solver. If SOLVER=ITERATIVE SCALING is selected, the pre-conditioning is limited to a scaling of the diagonal terms, SOLVER=ITERATIVE CHOLESKY triggers Incomplete Cholesky pre-conditioning. Cholesky pre-conditioning leads to a better convergence and maybe to shorter execution times, however, it requires additional storage roughly corresponding to the non-zeros in the matrix. If you are short of memory, diagonal scaling might be your last resort. The iterative methods perform well for truly three-dimensional structures. For instance, calculations for a hemisphere were about nine times faster with the ITERATIVE SCALING solver, and three times faster with the ITERATIVE CHOLESKY solver than with SPOOLES. For two-dimensional structures such as plates or shells, the performance might break down drastically and convergence often requires the use of Cholesky preconditioning. SPOOLES (and any of the other direct solvers) performs well in

most situations with emphasis on slender structures but requires much more storage than the iterative solver. PARDISO is the Intel proprietary solver.

The parameter DIRECT indicates that automatic incrementation should be switched off. The increments will have the fixed length specified by the user on the second line.

The parameter MAGNETOSTATICS indicates that only the steady state should be calculated. Since the magnetic field does not change, no heat is produced and a heat transfer analysis does not make sense. The loading (coil current in the shell elements) is applied by its full strength. If the MAGNETOSTATICS parameter is absent, the calculation is assumed to be time dependent and a transient analysis is performed. A transient analysis triggers by default a complementary heat transfer analysis, thus the temperature dependence of the properties of the materials involved must be provided. Here too, the coil currents are by default applied by their full strength at the start of the step. Other loading patterns can be defined by an *AMPLITUDE card.

The parameter DELTMX can be used to limit the temperature change in two subsequent increments. If the temperature change exceeds DELTMX the increment is restarted with a size equal to D_A times DELTMX divided by the temperature change. The default for D_A is 0.85, however, it can be changed by the *CONTROLS keyword. DELTMX is only active in transient calculations. Default value is 10^{30}.

The parameter TIME RESET can be used to force the total time at the end of the present step to coincide with the total time at the end of the previous step. If there is no previous step the targeted total time is zero. If this parameter is absent the total time at the end of the present step is the total time at the end of the previous step plus the time period of the present step (2nd parameter underneath the *HEAT TRANSFER keyword). Consequently, if the time at the end of the previous step is 10. and the present time period is 1., the total time at the end of the present step is 11. If the TIME RESET parameter is used, the total time at the beginning of the present step is 9. and at the end of the present step it will be 10. This is sometimes useful if transient heat transfer calculations are preceded by a stationary heat transfer step to reach steady state conditions at the start of the transient heat transfer calculations. Using the TIME RESET parameter in the stationary step (the first step in the calculation) will lead to a zero total time at the start of the subsequent instationary step.

The parameter TOTAL TIME AT START can be used to set the total time at the start of the step to a specific value.

Finally, the paramter NO HEAT TRANSFER may be used in a transient analysis to indicate that no heat generated by the Eddy currents should be calculated. However, an external temperature field may be defined using the *TEMPERATURE card.

First line:

- *ELECTROMAGNETICS
- Enter any needed parameters and their values.

Second line:

- Initial time increment. This value will be modified due to automatic incrementation, unless the parameter DIRECT was specified (default 1.).
- Time period of the step (default 1.).
- Minimum time increment allowed. Only active if DIRECT is not specified. Default is the initial time increment or 1.e-5 times the time period of the step, whichever is smaller.
- Maximum time increment allowed. Only active if DIRECT is not specified. Default is 1.e+30.

Example:

```
*ELECTROMAGNETICS,DIRECT
.1,1.
```

defines a static step and selects the SPOOLES solver as linear equation solver in the step (default). The second line indicates that the initial time increment is .1 and the total step time is 1. Furthermore, the parameter DIRECT leads to a fixed time increment. Thus, if successful, the calculation consists of 10 increments of length 0.1.

Example files: induction1.

7.40 *ELEMENT

Keyword type: model definition

With this option elements are defined. There is one required parameter, TYPE and one optional parameter, ELSET. The parameter TYPE defines the kind of element which is being defined. The following types can be selected:

- General 3D solids
  - C3D4 (4-node linear tetrahedral element)
  - C3D6 (6-node linear triangular prism element)
  - C3D8 (3D 8-node linear isoparametric element)
  - C3D8R (the C3D8 element with reduced integration)
  - C3D10 (10-node quadratic tetrahedral element)
  - C3D15 (15-node quadratic triangular prism element)
  - C3D20 (3D 20-node quadratic isoparametric element)
  - C3D20R (the C3D20 element with reduced integration)
- "ABAQUS" 3D solids for heat transfer (names are provided for compatibility)

  - DC3D4: identical to C3D4
  - DC3D6: identical to C3D6
  - DC3D8: identical to C3D8
  - DC3D10: identical to C3D10
  - DC3D15: identical to C3D15
  - DC3D20: identical to C3D20

- Shell elements
  - S6 (6-node triangular shell element)
  - S8 (8-node quadratic shell element)
  - S8R (the S8 element with reduced integration)

- Plane stress elements
  - CPS6 (6-node triangular plane stress element)
  - CPS8 (8-node quadratic plane stress element)
  - CPS8R (the CPS8 element with reduced integration)

- Plane strain elements
  - CPE6 (6-node triangular plane strain element)
  - CPE8 (8-node quadratic plane strain element)
  - CPE8R (the CPS8 element with reduced integration)

- Axisymmetric elements
  - CAX6 (6-node triangular axisymmetric element)
  - CAX8 (8-node quadratic axisymmetric element)
  - CAX8R (the CAX8 element with reduced integration)

- Beam elements
  - B32 (3-node beam element)
  - B32R (the B32 element with reduced integration)

- Special elements
  - D (3-node network element)
  - GAPUNI (2-node unidirectional gap element)

Notice that the S8, S8R, CPS8, CPS8R, CPE8, CPE8R, CAX8, CAX8R, B32 and B32R element are internally expanded into 20-node brick elements. Please have a look at Section 6.2 for details and decision criteria which element to take. The element choice determines to a large extent the quality of the results. Do not take element choice lightheartedly! The parameter ELSET is used to assign the elements to an element set. If the set already exists, the elements are ADDED to the set.

First line:

- *ELEMENT
- Enter any needed parameters and their values.

Following line:

- Element number.
- Node numbers forming the element. The order of nodes around the element is given in section 2.1. Use continuation lines for elements having more than 15 nodes (maximum 16 entries per line).

Repeat this line if needed.

Example:

```
*ELEMENT,ELSET=Eall,TYPE=C3D20R
1,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,
16,17,18,19,20
```

defines one 20-node element with reduced integration and stores it in set Eall.

Example files: beam8p, beam10p, beam20p.

7.41 *ELEMENT OUTPUT

Keyword type: step

This option is used to save selected element variables averaged at the nodal points in a frd file (extension .frd) for subsequent viewing by CalculiX GraphiX. The options and its use are identical with the *EL FILE keyword, however, the resulting .frd file is a mixture of binary and ASCII (the .frd file generated by using *EL FILE is completely ASCII). This has the advantage that the file is smaller and can be faster read by cgx..

Example:

```
*ELEMENT OUTPUT
S,PEEQ
```

requests that the (Cauchy) stresses and the equivalent plastic strain is stored in .frd format for subsequent viewing with CalculiX GraphiX.

Example files: cubespring.

7.42 *EL FILE

Keyword type: step

This option is used to save selected element variables averaged at the nodal points in a frd file (extension .frd) for subsequent viewing by CalculiX GraphiX. The following element variables can be selected (the label is square brackets [] is the one used in the .frd file; for frequency calculations with cyclic symmetry both a real and an imaginary part may be stored, in all other cases only the real part is stored):

- CEEQ [PE]: equivalent creep strain (is converted internally into PEEQ since the viscoplastic theory does not distinguish between the two; consequently, the user will find PEEQ in the frd file, not CEEQ)
- E [TOSTRAIN (real),TOSTRAII (imaginary)]: strain. This is the total Lagrangian strain for (hyper)elastic materials and incremental plasticity and the total Eulerian strain for deformation plasticity.
- ECD [CURR]: electrical current density. This only applies to electromagnetic calculations.
- ENER [ENER]: the energy density.
- ERR [ERROR (real), ERRORI (imaginary)]: Extrapolation error estimator for stress calculations (cf. Section 6.12). Notice that ERR and ZZS are mutually exclusive.
- HER [HERROR (real), HERRORI (imaginary)]: Extrapolation error estimator for heat transfer (cf. Section 6.12).
- HFL [FLUX]: heat flux in structures.
- HFLF: heat flux in CFD-calculations.
- MAXE [MSTRAIN]: maximum of the absolute value of the worst principal strain at all times for *FREQUENCY calculations with cyclic symmetry. It is stored for nodes belonging to the node set with name STRAINDOMAIN. This node set must have been defined by the user with the *NSET command. The worst principal strain is the maximum of the absolute value of the principal strains times its original sign.
- MAXS [MSTRESS]: maximum of the absolute value of the worst principal stress at all times for *FREQUENCY calculations with cyclic symmetry. It is stored for nodes belonging to the node set with name STRESSDOMAIN. This node set must have been defined by the user with the *NSET

command. The worst principal stress is the maximum of the absolute value of the principal stresses times its original sign.

- ME [MESTRAIN (real), MESTRAII (imaginary)]: strain. This is the mechanical Lagrangian strain for (hyper)elastic materials and incremental plasticity and the mechanical Eulerian strain for deformation plasticity (mechanical strain = total strain - thermal strain).
- PEEQ [PE]: equivalent plastic strain.
- PHS [PSTRESS]: stress: magnitude and phase (only for *STEADY STATE DYNAMICS calculations and *FREQUENCY calculations with cyclic symmetry).
- S [STRESS (real), STRESSI (imaginary)]: true (Cauchy) stress in structures. For beam elements this tensor is replaced by the section forces if SECTION FORCES is selected.
- SF: total stress in CFD-calculations.
- SVF: viscous stress in CFD-calculations.
- SDV [SDV]: the internal state variables.
- ZZS [ZZSTR (real), ZZSTRI (imaginary)]: Zienkiewicz-Zhu improved stress [80], [81](cf. Section 6.12). Notice that ZZS and ERR are mutually exclusive.

The selected variables are stored for the complete model. Due to the averaging process jumps at material interfaces are smeared out unless you model the materials on both sides of the interface independently and connect the coinciding nodes with MPC's.

For frequency calculations with cyclic symmetry the eigenmodes are generated in pairs (different by a phase shift of 90 degrees). Only the first one of each pair is stored in the frd file. If S is selected (the stresses) two load cases are stored in the frd file: a loadcase labeled STRESS containing the real part of the stresses and a loadcase labeled STRESSI containing the imaginary part of the stresses. For all other variables only the real part is stored.

The key ENER triggers the calculation of the internal energy. If it is absent no internal energy is calculated. Since in nonlinear calculations the internal energy at any time depends on the accumulated energy at all previous times, the selection of ENER in nonlinear calculations (geometric or material nonlinearities) must be made in the first step.

The first occurrence of an *EL FILE keyword card within a step wipes out all previous element variable selections for file output. If no *EL FILE card is used within a step the selections of the previous step apply. If there is no previous step, no element variables will be stored.

There are eight optional parameters: FREQUENCY, FREQUENCYF, GLOBAL, OUTPUT, SECTION FORCES, TIME POINTS, NSET and CONTACT ELEMENTS. The parameters FREQUENCY and TIME POINTS are mutually exclusive.

FREQUENCY applies to nonlinear calculations where a step can consist of several increments. Default is FREQUENCY=1, which indicates that the results of all increments will be stored. FREQUENCY=N with N an integer indicates that the results of every Nth increment will be stored. The final results of a step are always stored. If you only want the final results, choose N very big. The value of N applies to *OUTPUT,*ELEMENT OUTPUT, *EL FILE, *ELPRINT, *NODE OUTPUT, *NODE FILE, *NODE PRINT, *FACE PRINT ,*CONTACT OUTPUT, *CONTACT FILE and *CONTACT PRINT. If the FREQUENCY parameter is used for more than one of these keywords with conflicting values of N, the last value applies to all. A frequency parameter stays active across several steps until it is overwritten by another FREQUENCY value or the TIME POINTS parameter.

The 3D fluid analogue of FREQUENCY is FREQUENCYF. In coupled calculations FREQUENCY applies to the thermomechanical output, FREQUENCYF to the 3D fluid output.

With the parameter GLOBAL you tell the program whether you would like the results in the global rectangular coordinate system or in the local element system. If an *ORIENTATION card is applied to the element at stake, this card defines the local system. If no *ORIENTATION card is applied to the element, the local system coincides with the global rectangular system. Default value for the GLOBAL parameter is GLOBAL=YES, which means that the results are stored in the global system. If you prefer the results in the local system, specify GLOBAL=NO.

The parameter OUTPUT can take the value 2D or 3D. This has only effect for 1d and 2d elements such as beams, shells, plane stress, plane strain and axisymmetric elements AND provided it is used in the first step. If OUTPUT=3D, the 1d and 2d elements are stored in their expanded three-dimensional form. In particular, the user has the advantage to see his/her 1d/2d elements with their real thickness dimensions. However, the node numbers are new and do not relate to the node numbers in the input deck. Once selected, this parameter is active in the complete calculation. If OUTPUT=2D the fields in the expanded elements are averaged to obtain the values in the nodes of the original 1d and 2d elements. In particular, averaging removes the bending stresses in beams and shells. Therefore, default for beams and shells is OUTPUT=3D, for plane stress, plane strain and axisymmetric elements it is OUTPUT=2D.

The selection of SECTION FORCES makes sense for beam elements only. Furthermore, SECTION FORCES and OUTPUT=3D are mutually exclusive (if both are used the last prevails). If selected, the stresses in the beam nodes are replaced by the section forces. They are calculated in a local coordinate system consisting of the 1-direction $\mathbf{n_1}$, the 2-direction $\mathbf{n_2}$ and 3-direction or tangential direction $\mathbf{t}$ (Figure 66). Accordingly, the stress components now have the following meaning:

- xx: Shear force in 1-direction
- yy: Shear force in 2-direction

- zz: Normal force
- xy: Moment about the 1-direction
- xz: Moment about the 2-direction
- yz: Torque

For all elements except the beam elements the parameter SECTION FORCES has no effect. If SECTION FORCES is not selected the stress tensor is averaged across the beam section.

With the parameter TIME POINTS a time point sequence can be referenced, defined by a *TIME POINTS keyword. In that case, output will be provided for all time points of the sequence within the step and additionally at the end of the step. No other output will be stored and the FREQUENCY parameter is not taken into account. Within a step only one time point sequence can be active. If more than one is specified, the last one defined on any of the keyword cards *NODE FILE, *EL FILE, *NODE PRINT or *EL PRINT will be active. The TIME POINTS option should not be used together with the DIRECT option on the procedure card. The TIME POINTS parameters stays active across several steps until it is replaced by another TIME POINTS value or the FREQUENCY parameter.

The specification of a node set with the parameter NSET limits the output to the nodes contained in the set. Remember that the frd file is node based, so element results are also stored at the nodes after extrapolation from the integration points. For cyclic symmetric structures the usage of the parameter NGRAPH on the *CYCLIC SYMMETRY MODEL card leads to output of the results not only for the node set specified by the user (which naturally belongs to the base sector) but also for all corresponding nodes of the sectors generated by the NGRAPH parameter. Notice that for cyclic symmetric structures the use of NSET is mandatory.

Finally, the parameter CONTACT ELEMENTS stores the contact elements which have been generated in each iteration in a file with the name contactelements.inp. When opening the frd file with CalculiX GraphiX these files can be read with the command “read contactelements.inp” and visualized by plotting the elements in the sets contactelements_stα_inβ_atγ_itδ, where α is the step number, β the increment number, γ the attempt number and δ the iteration number.

First line:

- *EL FILE
- Enter any needed parameters and their values.

Second line:

- Identifying keys for the variables to be printed, separated by commas.

```
Example:

*EL FILE
S,PEEQ
```

requests that the (Cauchy) stresses and the equivalent plastic strain is stored in .frd format for subsequent viewing with CalculiX GraphiX.

Example files: beamt, fullseg, segment1, segdyn.

7.43 *EL PRINT

Keyword type: step

This option is used to print selected element variables in an ASCII file with the name jobname.dat. Some of the element variables are printed in the integration points, some are whole element variables. The following variables can be selected:

- Integration point variables
  - true (Cauchy) stress in structures (key=S).
  - viscous stress in CFD calculations (key=SVF).
  - strain (key=E). This is the total Lagrangian strain for (hyper)elastic materials and incremental plasticity and the total Eulerian strain for deformation plasticity.
  - strain (key=ME). This is the mechanical Lagrangian strain for (hyper)elastic materials and incremental plasticity and the mechanical Eulerian strain for deformation plasticity (mechanical strain = total strain - thermal strain).
  - equivalent plastic strain (key=PEEQ)
  - equivalent creep strain (key=CEEQ; is converted internally into PEEQ since the viscoplastic theory does not distinguish between the two; consequently, the user will find PEEQ in the dat file, not CEEQ)
  - the energy density (key=ENER)
  - the internal state variables (key=SDV)
  - heat flux (key=HFL). This also applies to CFD-calculations involving heat transfer.
- Whole element variables
  - the internal energy (key=ELSE)
  - the kinetic energy (key=ELKE)
  - the volume (key=EVOL)

The keys ENER and ELSE trigger the calculation of the internal energy. If they are absent no internal energy is calculated. Since in nonlinear calculations the internal energy at any time depends on the accumulated energy at all previous times, the selection of ENER and/or ELSE in nonlinear calculations (geometric or material nonlinearities) must be made in the first step.

There are six parameters, ELSET, FREQUENCY, FREQUENCYF, TOTALS, GLOBAL and TIME POINTS. The parameter ELSET is required, defining the set of elements for which these stresses should be printed. If this card is omitted, no values are printed. Several *EL PRINT cards can be used within one and the same step.

The parameters FREQUENCY and TIME POINTS are mutually exclusive.

The FREQUENCY parameter is optional and applies to nonlinear calculations where a step can consist of several increments. Default is FREQUENCY=1, which indicates that the results of all increments will be stored. FREQUENCY=N with N an integer indicates that the results of every Nth increment will be stored. The final results of a step are always stored. If you only want the final results, choose N very big. The value of N applies to *OUTPUT,*ELEMENT OUTPUT, *EL FILE, *ELPRINT, *NODE OUTPUT, *NODE FILE, *NODE PRINT, *FACE PRINT,*CONTAC *CONTACT FILE and *CONTACT PRINT. If the FREQUENCY parameter is used for more than one of these keywords with conflicting values of N, the last value applies to all. A frequency parameter stays active across several steps until it is overwritten by another FREQUENCY value or the TIME POINTS parameter.

The 3D fluid analogue of FREQUENCY is FREQUENCYF. In coupled calculations FREQUENCY applies to the thermomechanical output, FREQUENCYF to the 3D fluid output.

The optional parameter TOTALS only applies to whole element variables. If TOTALS=YES the sum of the variables for the whole element set is printed in addition to their value for each element in the set separately. If TOTALS=ONLY is selected the sum is printed but the individual element contributions are not. If TOTALS=NO (default) the individual contributions are printed, but their sum is not.

With the parameter GLOBAL (optional) you tell the program whether you would like the results in the global rectangular coordinate system or in the local element system. If an *ORIENTATION card is applied to the element at stake, this card defines the local system. If no *ORIENTATION card is applied to the element, the local system coincides with the global rectangular system. Default value for the GLOBAL parameter is GLOBAL=NO, which means that the results are stored in the local system. If you prefer the results in the global system, specify GLOBAL=YES.

With the parameter TIME POINTS a time point sequence can be referenced, defined by a *TIME POINTS keyword. In that case, output will be provided for all time points of the sequence within the step and additionally at the end of the step. No other output will be stored and the FREQUENCY parameter is not taken into account. Within a step only one time point sequence can be active. If more than one is specified, the last one defined on any of the keyword cards

*NODE FILE, *EL FILE, *NODE PRINT, *EL PRINT or *FACE PRINT will be active. The TIME POINTS option should not be used together with the DIRECT option on the procedure card. The TIME POINTS parameters stays active across several steps until it is replaced by another TIME POINTS value or the FREQUENCY parameter.

The first occurrence of an *EL FILE keyword card within a step wipes out all previous element variable selections for print output. If no *EL FILE card is used within a step the selections of the previous step apply, if any.

First line:

- *EL PRINT
- Enter the parameter ELSET and its value.

Second line:

- Identifying keys for the variables to be printed, separated by commas.

```
Example:

*EL PRINT,ELSET=Copper
E
```

requests to store the strains at the integration points in the elements of set Copper in the .dat file.

Example files: beampt, beamrb, beamt4.

7.44 *ELSET

Keyword type: model definition

This option is used to assign elements to an element set. The parameter ELSET containing the name of the set is required (maximum 80 characters), whereas the parameter GENERATE (without value) is optional. If present, element ranges can be expressed by their initial value, their final value, and an increment. If a set with the same name already exists, it is reopened and complemented. The name of a set is case insensitive. Internally, it is modified into upper case and a 'E' is appended to denote it as element set.

First line:

- *ELSET
- Enter any needed parameters and their values.

Following line if the GENERATE parameter is omitted:

- List of elements and/or sets of elements previously defined to be assigned to this element set (maximum 16 entries per line).

Repeat this line if needed.

Following line if the GENERATE parameter is included:

- First element in set.
- Last element in set.
- Increment in element numbers between elements in the set. Default is 1.

Repeat this line if needed.

```
Example:

*ELSET,ELSET=E1,GENERATE
20,25
*ELSET,ELSET=E2
E1,50,51
```

assigns the elements with numbers 20, 21, 22, 23, 24 and 25 to element set E1 and the elements with numbers 20, 21, 22, 23, 24, 25 (= set E1), 50 and 51 to element set E2.

Example files: segment, beampo1, beampset.

7.45 *END STEP

Keyword type: step

This option concludes the definition of a step.

First and only line:

- *END STEP

```
Example:

*END STEP
```

concludes a step. Each *STEP card must at some point be followed by an *END STEP card.

Example files: beamstraight, beamt.

7.46 *EQUATION

Keyword type: model definition (no REMOVE parameter) and step (only for REMOVE)

With this option, a linear equation constraint between arbitrary displacement components at any nodes where these components are active can be imposed. The equation is assumed to be homogeneous, and all variables are to be

written on the left hand side of the equation. The first variable is considered to be the dependent one, and is subsequently eliminated from the equation, i.e. the corresponding degree of freedom does not show up in the stiffness matrix. This reduces the size of the matrix. A degree of freedom in a node can only be used once as the dependent node in an equation or in a SPC. For CFD-applications it is important for the stability of the calculation that the coefficient of the dependent degree of freedom is as large as possible compared to the coefficients of the independent degrees of freedom. For instance, setting the radial velocity orthogonal to the z-axis to zero corresponds to a MPC linking the x- and y-component of the velocity. The component with the largest coefficient should be chosen as dependent degree of freedom.

There are two optional parameters: REMOVE and REMOVE ALL. The parameter REMOVE can be used to remove equations corresponding with selected dependent degrees of freedom. These are listed underneath the *EQUATION keyword by node number, first degree of freedom and last degree of freedom. This triggers the deletion of all equations for which the dependent degree of freedom corresponds to the range from the first to the last degree of freedom of the selected node. If the last degree of freedom was omitted, it equals the first degree of freedom.

The parameter REMOVE ALL is used to remove all equations. Notice that the latter option removes all linear and nonlinear equations, irrespective whether they were defined with a *EQUATION card, a *MPC card or whether they were generated internally. Use of the REMOVE or the REMOVE ALL parameter usually makes sense only in step 2 or higher.

First line:

- *EQUATION
- one of the optional parameters, if applicable

Following lines in the absence of the REMOVE and REMOVE ALL parameter, in a set: First line of set:

- Number of terms in the equation.

Following lines of set (maximum 12 entries per line):

- Node number of the first variable.
- Degree of freedom at above node for the first variable.
- Value of the coefficient of the first variable.
- Node number of the second variable.
- Degree of freedom at above node for the second variable.
- Value of the coefficient of the second variable.

- Etc..

Continue, giving node number, degree of freedom, value of the coefficient, etc. Repeat the above line as often as needed if there are more than four terms in the *EQUATION. Specify exactly four terms per line for each constraint, except for the last line which may have less than four terms.

Following lines if the REMOVE parameter was selected:

- Node number or Node set label
- First degree of freedom
- Last degree of freedom (optional)

Repeat this line if needed.

If the REMOVE ALL parameter was selected no additional lines are necessary.

```
Example:

*EQUATION
3
3,2,2.3,28,1,4.05,17,1,-8.22
```

defines an equation of the form $2.3v_3 + 4.05u_{28} - 8.22u_{17} = 0$, where u, v and w are the displacement for degree of freedom one, two and three, respectively.

```
Example:

*EQUATION,REMOVE
10,1,3
```

removes all equations for which the dependent degree of freedom corresponds to the degrees of freedom 1, 2 or 3 of node 10.

Example files: achtel2, achtel29, achtel9, achtelcas, beamnlmpc, equrem1, equrem2, equrem3.

7.47 *EXPANSION

Keyword type: model definition, material

This option is used to define the thermal expansion coefficients of a material. They are interpreted as total expansion coefficients with respect to a reference temperature T_{ref}, i.e. the thermal strain ϵ_{th} of a material at a final temperature T and with initial temperature T_0 is determined by

$$\epsilon_{th} = \alpha(T)(T - T_{ref}) - \alpha(T_o)(T_o - T_{ref}), \tag{336}$$

where $\alpha(T)$ is the thermal coefficient at a temperature T. There are two optional parameters TYPE and ZERO. Default for TYPE is TYPE=ISO, other

values are TYPE=ORTHO for orthotropic materials and TYPE=ANISO for anisotropic materials. All constants may be temperature dependent. The parameter ZERO is used to determine the reference temperature, default is 0.

First line:

- *EXPANSION
- Enter the TYPE and ZERO parameters and their values, if needed

Following line for TYPE=ISO:

- α.
- Temperature.

Repeat this line if needed to define complete temperature dependence.
Following line for TYPE=ORTHO:

- α_{11}.
- α_{22}.
- α_{33}.
- Temperature.

Repeat this line if needed to define complete temperature dependence.
Following line for TYPE=ANISO:

- α_{11}.
- α_{22}.
- α_{33}.
- α_{12}.
- α_{13}.
- α_{23}.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

`Example:`

```
*EXPANSION,ZERO=273.
12.E-6,373.
20.E-6,573.
```

tells you that the thermal strain in a body made of this material is $100. \times 12. \times 10^{-6} = 12. \times 10^{-4}$ if heated from T=273 to T=373, and $300 \times 20 \times 10^{-6} = 60 \times 10^{-4}$ if heated from T=273 to T=573.

Example files: beamt, beamt2.

7.48 *FACE PRINT

Keyword type: step

This option is used to print selected facial variables in file jobname.dat. The following variables can be selected:

- Fluid dynamic drag stresses (key=DRAG), only makes sense for 3D fluid calculations
- Heat flux (key=FLUX), only makes sense for heat calculations (structural or CFD)

The drag stresses are printed in the integration points of the faces. The output lists the element, the local face number, the integration point, the x-, y- and z- component of the surface stress vector in the global coordinate system, the normal component, the shear component and the global coordinates of the integration point. At the end of the listing the surface stress vectors are integrated to yield the total force on the surface.

The heat flux is also printed in the integration points of the faces. The output lists the element, the local face number, the integration point, the heat flux (positive = flux leaving the element through the surface defined by the parameter SURFACE) and the global coordinates of the integration point. At the end of the listing the heat flux vectors are integrated to yield the total heat flow through the surface.

There are three parameters, FREQUENCYF, SURFACE and TIME POINTS. The parameter SURFACE is required, defining the facial surface for which the drag stresses are to be printed. If this card is omitted, no values are printed. Several *FACE PRINT cards can be used within one and the same step.

The parameters FREQUENCYF and TIME POINTS are mutually exclusive.

The parameter FREQUENCYF is optional, and applies to nonlinear calculations where a step can consist of several increments. Default is FREQUENCYF=1, which indicates that the results of all increments will be stored. FREQUENCYF=N with N an integer indicates that the results of every Nth increment will be stored. The final results of a step are always stored. If you only want the final results, choose N very big. The value of N applies to *OUTPUT,*ELEMENT OUTPUT, *EL FILE, *ELPRINT, *NODE OUTPUT, *NODE FILE, *NODE PRINT, *FACE PRINT,*CONTACT OUTPUT, *CONTACT FILE and *CONTACT PRINT. If the FREQUENCYF parameter is used for more than one of these keywords with conflicting values of N, the last value applies to all. A FREQUENCYF parameter stays active across several steps until it is overwritten by another FREQUENCYF value or the TIME POINTS parameter.

With the parameter TIME POINTS a time point sequence can be referenced, defined by a *TIME POINTS keyword. In that case, output will be provided for all time points of the sequence within the step and additionally at the end of the step. No other output will be stored and the FREQUENCYF parameter is not taken into account. Within a step only one time point sequence can

be active. If more than one is specified, the last one defined on any of the keyword cards *NODE FILE, *EL FILE, *NODE PRINT or *EL PRINT will be active. The TIME POINTS option should not be used together with the DIRECT option on the procedure card. The TIME POINTS parameters stays active across several steps until it is replaced by another TIME POINTS value or the FREQUENCYF parameter.

The first occurrence of an *FACE PRINT keyword card within a step wipes out all previous facial variable selections for print output. If no *FACE PRINT card is used within a step the selections of the previous step apply, if any.

First line:

- *FACE PRINT
- Enter the parameter SURFACE and its value.

Second line:

- Identifying keys for the variables to be printed, separated by commas.

Example:

```
*FACE PRINT,SURFACE=S1
DRAG
```

requests the storage of the drag stresses for the faces belonging to (facial) set N1 in the .dat file.

Example files: fluid2.

7.49 *FILM

Keyword type: step

This option allows the specification of film heat transfer. This is convective heat transfer of a surface at temperature T and with film coefficient h to the environment at temperature T_0. The environmental temperature T_0 is also called the sink temperature. The convective heat flux q satisfies:

$$q = h(T - T_0). \tag{337}$$

In order to specify which face the flux is entering or leaving the faces are numbered. The numbering depends on the element type.

For hexahedral elements the faces are numbered as follows (numbers are node numbers):

- Face 1: 1-2-3-4
- Face 2: 5-8-7-6
- Face 3: 1-5-6-2

- Face 4: 2-6-7-3
- Face 5: 3-7-8-4
- Face 6: 4-8-5-1

for tetrahedral elements:

- Face 1: 1-2-3
- Face 2: 1-4-2
- Face 3: 2-4-3
- Face 4: 3-4-1

and for wedge elements:

- Face 1: 1-2-3
- Face 2: 4-5-6
- Face 3: 1-2-5-4
- Face 4: 2-3-6-5
- Face 5: 3-1-4-6

for quadrilateral plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-4
- Face 4: 4-1
- Face N: in negative normal direction (only for plane stress)
- Face P: in positive normal direction (only for plane stress)

for triangular plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-1
- Face N: in negative normal direction (only for plane stress)
- Face P: in positive normal direction (only for plane stress)

for quadrilateral shell elements:

- Face NEG or 1: in negative normal direction
- Face POS or 2: in positive normal direction
- Face 3: 1-2
- Face 4: 2-3
- Face 5: 3-4
- Face 6: 4-1

for triangular shell elements:

- Face NEG or 1: in negative normal direction
- Face POS or 2: in positive normal direction
- Face 3: 1-2
- Face 4: 2-3
- Face 5: 3-1

The labels NEG and POS can only be used for uniform, non-forced convection and are introduced for compatibility with ABAQUS. Notice that the labels 1 and 2 correspond to the brick face labels of the 3D expansion of the shell (Figure 61).

for beam elements:

- Face 1: in negative 1-direction
- Face 2: in positive 1-direction
- Face 3: in positive 2-direction
- Face 5: in negative 2-direction

The beam face numbers correspond to the brick face labels of the 3D expansion of the beam (Figure 66).

Film flux characterized by a uniform film coefficient is entered by the distributed flux type label Fx where x is the number of the face, followed by the sink temperature and the film coefficient. If the film coefficient is nonuniform the label takes the form FxNUy and a user subroutine film.f must be provided specifying the value of the film coefficient and the sink temperature. The label can be up to 20 characters long. In particular, y can be used to distinguish different nonuniform film coefficient patterns (maximum 16 characters).

In case the element face is adjacent to a moving fluid the temperature of which is also unknown (forced convection), the distributed flux type label is FxFC where x is the number of the face. It is followed by the fluid node number it exchanges convective heat with and the film coefficient. To define a nonuniform film coefficient the label FxFCNUy must be used and a subroutine film.f

defining the film coefficient be provided. The label can be up to 20 characters long. In particular, y can be used to distinguish different nonuniform film coefficient patterns (maximum 14 characters).

Optional parameters are OP, AMPLITUDE, TIME DELAY, FILM AMPLITUDE and FILM TIME DELAY. OP takes the value NEW or MOD. OP=MOD is default and implies that the film fluxes on different faces are kept over all steps starting from the last perturbation step. Specifying a film flux on a face for which such a flux was defined in a previous step replaces this value. OP=NEW implies that all previous film flux is removed. If multiple *FILM cards are present in a step this parameter takes effect for the first *FILM card only.

The AMPLITUDE parameter allows for the specification of an amplitude by which the sink temperature is scaled (mainly used for dynamic calculations). Thus, in that case the sink temperature values entered on the *FILM card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference value is replaced by the actual value at that time. In subsequent steps this value is kept constant unless it is explicitly redefined or the amplitude is defined using TIME=TOTAL TIME in which case the amplitude keeps its validity. The AMPLITUDE parameter has no effect on nonuniform and forced convective fluxes.

The TIME DELAY parameter modifies the AMPLITUDE parameter. As such, TIME DELAY must be preceded by an AMPLITUDE name. TIME DELAY is a time shift by which the AMPLITUDE definition it refers to is moved in positive time direction. For instance, a TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The TIME DELAY parameter must only appear once on one and the same keyword card.

The FILM AMPLITUDE parameter allows for the specification of an amplitude by which the film coefficient is scaled (mainly used for dynamic calculations). Thus, in that case the film coefficient values entered on the *FILM card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference value is replaced by the actual value at that time, for use in subsequent steps. The FILM AMPLITUDE parameter has no effect on nonuniform fluxes.

The FILM TIME DELAY parameter modifies the FILM AMPLITUDE parameter. As such, FILM TIME DELAY must be preceded by an FILM AMPLITUDE name. FILM TIME DELAY is a time shift by which the FILM AMPLITUDE definition it refers to is moved in positive time direction. For instance, a FILM TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The FILM TIME DELAY parameter must only appear once on one and the same keyword card.

First line:

- *FILM
- Enter any needed parameters and their value

Following line for uniform, explicit film conditions:

- Element number or element set label.
- Film flux type label (Fx).
- Sink temperature.
- Film coefficient.

Repeat this line if needed.
Following line for nonuniform, explicit film conditions:

- Element number or element set label.
- Film flux type label (FxNUy).

Repeat this line if needed.
Following line for forced convection with uniform film conditions:

- Element number or element set label.
- Film flux type label (FxFC).
- Fluid node.
- Film coefficient.

Repeat this line if needed.
Following line for forced convection with nonuniform film conditions:

- Element number or element set label.
- Film flux type label (FxFCNUy).
- Fluid node.

Repeat this line if needed.

`Example:`

```
*FILM
20,F1,273.,.1
```

assigns a film flux to face 1 of element 20 with a film coefficient of 0.1 and a sink temperature of 273.

Example files: oneel20fi.

7.50 *FLUID CONSTANTS

Keyword type: model definition, material

With this option the specific heat at constant pressure and the dynamic viscosity of a gas or liquid can be defined. These properties are required for fluid dynamic network calculations. They can be temperature dependent.

First line:

- *FLUID CONSTANTS

Following line:

- Specific heat at constant pressure.
- Dynamic viscosity.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Example:

```
*FLUID CONSTANTS
1.032E9,71.1E-13,100.
```

defines the specific heat and dynamic viscosity for air at 100 K in a unit system using N, mm, s and K: $c_p = 1.032 \times 10^9 \text{mm}^2/\text{s}^2\text{K}$ and $\mu = 71.1 \times 10^{-13} \text{Ns/mm}^2$.

Example files: linearnet, branch1, branch2.

7.51 *FLUID SECTION

Keyword type: model definition

This option is used to assign material properties to network element sets. The parameters ELSET and MATERIAL are required, the parameters TYPE and OIL are optional. The parameter ELSET defines the network element set to which the material specified by the parameter MATERIAL applies.

The parameter TYPE is only necessary in fluid dynamic networks in which the pressure and/or the mass flow are unknown in at least one node. In that case, the type of fluid section must be selected from the list in section 6.2.28 and the appropriate constants describing the section must be specified in the line(s) underneath the *FLUID SECTION keyword card, eight per line, except for the last line which can contain less.

Finally, the parameter OIL defines the material parameters used in two-phase flow in gas pipes, restrictors and branches. Its argument must be the name of a material defined using the *MATERIAL card.

First line:

- *FLUID SECTION
- Enter any needed parameters.

Following line (only necessary if TYPE was used):

- First constant
- Second constant
- etc (maximum eight constants on this line)

Repeat this line if more than eight constants are needed to describe the fluid section.

Example:

```
*FLUID SECTION,MATERIAL=NITROGEN,ELSET=Eall
```

assigns material NITROGEN to all elements in (element) set Eall.

Example:

```
*FLUID SECTION,MATERIAL=AIR,ELSET=Eall,TYPE=ORIFICE_PK_MS
3.14,0.1,2.,0.01,0.1
```

assigns material AIR to all elements in set Eall. The type of fluid section is an orifice with the c_d coefficient calculated following the formulas by Parker and Kercher [57], modified for the influence of the rotational velocity by McGreehan and Schotsch [46]. The area of the orifice is 3.14, the length is 0.1, the diameter is 2., the inlet corner radius is 0.01 and the pipe diameter ratio is 0.1.

Example files: furnace, beamhtfc, branch1.

7.52 *FREQUENCY

Keyword type: step

This procedure is used to determine eigenfrequencies and the corresponding eigenmodes of a structure. The frequency range of interest can be specified by entering its lower and upper value. However, internally only as many frequencies are calculated as requested in the first field beneath the *FREQUENCY keyword card. Accordingly, if the highest calculated frequency is smaller than the upper value of the requested frequency range, there is no guarantee that all eigenfrequencies within the requested range were calculated. If the PERTURBATION parameter is used in the *STEP card, the load active in the last *STATIC step, if any, will be taken as preload. Otherwise, no preload will be active.

There are four optional parameters SOLVER, STORAGE, GLOBAL and CYCMPC. SOLVER specifies which solver is used to perform a decomposition

of the linear equation system. This decomposition is done only once. It is repeatedly used in the iterative procedure determining the eigenvalues. The following solvers can be selected:

- the SGI solver
- PARDISO
- SPOOLES [3, 4].
- TAUCS
- MATRIXSTORAGE. This is not really a solver. Rather, it is an option allowing the user to store the stiffness and mass matrix.

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, no eigenvalue analysis can be performed.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU decomposition, however, I was not able to run either of them so far. PARDISO is the Intel proprietary solver.

If the MATRIXSTORAGE option is used, the stiffness and mass matrices are stored in files jobname.sti and jobname.mas, respectively. These are ASCII files containing the nonzero entries (occasionally, they can be zero; however, none of the entries which are not listed are nonzero). Each line consists of two integers and one real: the row number, the column number and the corresponding value. The entries are listed column per column. In addition, a file jobname.dof is created. It has as many entries as there are rows and columns in the stiffness and mass matrix. Each line contains a real number of the form "a.b". Part a is the node number and b is the global degree of freedom corresponding to selected row. Notice that the program stops after creating these files. No further steps are treated. Consequently, *FREQUENCY, MATRIXSTORAGE only makes sense as the last step in a calculation.

The parameter STORAGE indicates whether the eigenvalues, eigenmodes, mass and stiffness matrix should be stored in binary form in file jobname.eig for further use in a *MODAL DYNAMICS or *STEADY STATE DYNAMICS procedure. Default is STORAGE=NO. Specify STORAGE=YES if storage is requested.

The parameters GLOBAL and CYCMPC only make sense in the presence of SOLVER=MATRIXSTORAGE. GLOBAL indicates whether the matrices should be stored in global coordinates, irrespective of whether a local coordinates system for any of the nodes in the structure was defined. Default is

GLOBAL=YES. For GLOBAL=NO the matrices are stored in local coordinates and the directions in file jobname.dof are local directions. Notice that the GLOBAL=NO only works if no single or multiple point constrains were defined and one and the same coordinate system was defined for ALL nodes in the structure. The second parameter (CYCMPC) specifies whether any cyclic multiple point constraints should remain active while assembling the stiffness and mass matrix before storing them. Default is CYCMPC=ACTIVE. CYCMPC=INACTIVE means that all cyclic MPC's and any other MPC's containing dependent nodes belonging to cyclic MPC's are removed before assembling the matrices. The CYCMPC parameter only makes sense if GLOBAL=YES, since only then are MPC's allowed.

For the iterative eigenvalue procedure ARPACK [41] is used. The eigenfrequencies are always stored in file jobname.dat.

At the start of a frequency calculation all single point constraint boundary conditions, which may be zero due to previous steps, are set to zero.

First line:

- *FREQUENCY

Second line:

- Number of eigenfrequencies desired.
- Lower value of requested eigenfrequency range (in cycles/time; default:0).
- Upper value of requested eigenfrequency range (in cycles/time; default: ∞).

```
Example:

*FREQUENCY
10
```

requests the calculation of the 10 lowest eigenfrequencies and corresponding eigenmodes.

Example files: beam8f, beamf.

7.53 *FRICTION

Keyword type: model definition, surface interaction

With this option the friction behavior of a surface interaction can be defined. The friction behavior is optional for contact analyses. There are no parameters.

The frictional behavior defines the relationship between the shear stress in the contact area and the relative tangential displacement between the slave and the master surface. It is characterized by a linear range with tangent λ (stick slope) for small relative displacements (stick) followed by a horizontal upper

bound (slip) given by μp, where μ is the friction coefficient and p the local pressure (Figure 115). μ is dimensionless and usually takes values between 0.1 and 0.5, λ has the dimension of force per volume and should be chosen to be about 10 times smaller than the spring constant.

For face-to-face penalty contact with PRESSURE-OVERCLOSURE=TIED the value of the friction coefficient is irrelevant.

First line:

- *FRICTION

Following line for all types of analysis except modal dynamics:

- $\mu(> 0)$.
- $\lambda(> 0)$.

Example:

```
*FRICTION
0.2,5000.
```

defines a friction coefficient of 0.2 and a stick slope of 5000.

Example files: friction1, friction2.

7.54 *GAP

Keyword type: model definition

This option is used to define a gap geometry. The parameter ELSET is required and defines the set of gap elements to which the geometry definition applies. Right now, all gap elements must be of the GAPUNI type and can be defined by an *ELEMENT card. The gap geometry is defined by its clearance d and direction $\boldsymbol{n}$ (a vector of length 1). Let the displacement vector of the first node of a GAPUNI element be $\boldsymbol{u_1}$ and the displacement vector of the second node $\boldsymbol{u_2}$. Then, the gap condition is defined by:

$$d + \boldsymbol{n} \cdot (\boldsymbol{u_2} - \boldsymbol{u_1}) \geq 0. \tag{338}$$

A *GAP card automatically triggers a geometrically nonlinear calculation, i.e. the NLGEOM parameter on the *STEP card is automatically triggered.

First line:

- *GAP
- Enter the ELSET parameter and its value.

Second line :

- gap clearance
- first component of the normalized gap direction
- second component of the normalized gap direction
- third component of the normalized gap direction

Example:

```
*GAP,ELSET=E1
0.5,0.,1.,0.
```

defines a clearance of 0.5 and the global y-axis as gap direction for all gap elements contained in element set E1.

Example files: gap.

7.55 *GAP CONDUCTANCE

Keyword type: model definition, surface interaction

This option allows for the definition of the conductance across a contact pair. The conductance is the ratio of the heat flow across the contact location and the temperature difference between the corresponding slave and master surface. Right now, gap conductance is only taken into account for penalty contact. The gap conductance is a property of the nonlinear contact spring elements generated during contact. This means that heat flow will only take place at those slave nodes, at which a contact spring element was generated. Whether or not a contact spring element is generated depends on the pressure-overclosure relationship on the *SURFACE BEHAVIOR card.

- if the pressure-overclosure relationship is linear or tabular a contact spring element is generated if the gap clearance does not exceed $c_0\sqrt{A}$, where A is the representative area at the slave node, or 10^{-10} if this area is zero (can happen for 2-dimensional elements). Default for c_0 is 10^{-3}, its value can be changed for a linear pressure-overclosure relationship.
- if the pressure-overclosure relationship is exponential a contact spring area is generated if the gap clearance does not exceed c_0 (cf. *SURFACE BEHAVIOR).

The conductance coefficient can be defined as a function of the contact pressure and the mean temperature of slave and master surface. Alternatively, the conductance can be coded by the user in the user subroutine gapcon.f, cf Section 8.4.11. In the latter case the option USER must be used on the *GAP CONDUCTANCE card.

First line:

- *GAP CONDUCTANCE
- Enter the parameter USER if appropriate

Following sets of lines define the conductance coefficients in the absence of the USER parameter: First line in the first set:

- Conductance.
- Contact pressure.
- Temperature.

Use as many lines in the first set as needed to define the conductance versus pressure curve for this temperature.

Use as many sets as needed to define complete temperature dependence.

```
Example:

*GAP CONDUCTANCE
100.,,273.
```

defines a conductance coefficient with value 100. for all contact pressures and all temperatures.

Example files: .

7.56 *HEADING

Keyword type: model definition

The heading block allows for a short problem description for identification and retrieval purposes. This description is reproduced at the top of the output file.

First line:

- *HEADING

Following line:

- Description of the problem.

```
Example:

*HEADING
Cantilever beam under tension and bending.
```

gives a title to the problem.

Example files: beampt, segment1.

7.57 *HEAT TRANSFER

Keyword type: step

This procedure is used to perform a pure heat transfer analysis. A heat transfer analysis is always nonlinear since the material properties depend on the solution, i.e. the temperature.

There are nine optional parameters: SOLVER, DIRECT, STEADY STATE, FREQUENCY, MODAL DYNAMIC, STORAGE, DELTMX, TIME RESET and TOTAL TIME AT START.

SOLVER determines the package used to solve the ensuing system of equations. The following solvers can be selected:

- the SGI solver
- PARADISO
- SPOOLES [3, 4].
- TAUCS
- the iterative solver by Rank and Ruecker [60], which is based on the algorithms by Schwarz [64].

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, the default is the iterative solver, which comes with the CalculiX package.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU decomposition, however, I was not able to run either of them so far. Next comes the iterative solver. If SOLVER=ITERATIVE SCALING is selected, the pre-conditioning is limited to a scaling of the diagonal terms, SOLVER=ITERATIVE CHOLESKY triggers Incomplete Cholesky pre-conditioning. Cholesky pre-conditioning leads to a better convergence and maybe to shorter execution times, however, it requires additional storage roughly corresponding to the non-zeros in the matrix. If you are short of memory, diagonal scaling might be your last resort. The iterative methods perform well for truly three-dimensional structures. For instance, calculations for a hemisphere were about nine times faster with the ITERATIVE SCALING solver, and three times faster with the ITERATIVE CHOLESKY solver than with SPOOLES. For two-dimensional structures such as plates or shells, the performance might break down drastically and convergence often requires the use of Cholesky preconditioning. SPOOLES (and any of the other direct solvers) performs well in

most situations with emphasis on slender structures but requires much more storage than the iterative solver. PARDISO is the Intel proprietary solver.

The parameter DIRECT indicates that automatic incrementation should be switched off. The increments will have the fixed length specified by the user on the second line.

The parameter STEADY STATE indicates that only the steady state should be calculated. For such an analysis the loads are by default applied in a linear way. Other loading patterns can be defined by an *AMPLITUDE card. If the STEADY STATE parameter is absent, the calculation is assumed to be time dependent and a transient analysis is performed. For a transient analysis the specific heat of the materials involved must be provided and the loads are by default applied by their full strength at the start of the step.

In a static step, loads are by default applied in a linear way. Other loading patterns can be defined by an *AMPLITUDE card.

The parameter FREQUENCY indicates that a frequency calculation should be performed. In a frequency step the homogeneous governing equation is solved, i.e. no loading applies, and the corresponding eigenfrequencies and eigenmodes are determined. This option is especially useful if the heat transfer option is used as an alias for true Helmholtz-type problems, e.g. in acoustics. The option FREQUENCY cannot (yet) be applied to cyclic symmetry calculations.

The parameter MODAL DYNAMIC is used for dynamic calculations in which the response is built as a linear combination of the eigenmodes of the system. It must be preceded by a *HEAT TRANSFER, FREQUENCY,STORAGE=YES procedure, either in the same deck, or in a previous run, either of which leads to the creation of a file with name jobname.eig containing the eigenvalues and eigenmodes of the system. A MODAL DYNAMIC procedure is necessarily linear and ideally suited of problems satisfying the classical wave equation (Helmholtz problem characterized by a second derivative in time, thus exhibiting a hyperbolic behavior), e.g linear acoustics.

The parameter STORAGE indicates whether the eigenvalues, eigenmodes, mass and stiffness matrix should be stored in binary form in file jobname.eig for further use in a *MODAL DYNAMICS or *STEADY STATE DYNAMICS procedure. Default is STORAGE=NO. Specify STORAGE=YES if storage is requested.

The parameter DELTMX can be used to limit the temperature change in two subsequent increments. If the temperature change exceeds DELTMX the increment is restarted with a size equal to D_A times DELTMX divided by the temperature change. The default for D_A is 0.85, however, it can be changed by the *CONTROLS keyword. DELTMX is only active in transient calculations. Default value is 10^{30}.

The parameter TIME RESET can be used to force the total time at the end of the present step to coincide with the total time at the end of the previous step. If there is no previous step the targeted total time is zero. If this parameter is absent the total time at the end of the present step is the total time at the end of the previous step plus the time period of the present step (2nd parameter

underneath the *HEAT TRANSFER keyword). Consequently, if the time at the end of the previous step is 10. and the present time period is 1., the total time at the end of the present step is 11. If the TIME RESET parameter is used, the total time at the beginning of the present step is 9. and at the end of the present step it will be 10. This is sometimes useful if transient heat transfer calculations are preceded by a stationary heat transfer step to reach steady state conditions at the start of the transient heat transfer calculations. Using the TIME RESET parameter in the stationary step (the first step in the calculation) will lead to a zero total time at the start of the subsequent instationary step.

Finally, the parameter TOTAL TIME AT START can be used to set the total time at the start of the step to a specific value.

First line:

- *HEAT TRANSFER
- Enter any needed parameters and their values.

Second line if FREQUENCY nor MODAL DYNAMIC is not selected:

- Initial time increment. This value will be modified due to automatic incrementation, unless the parameter DIRECT was specified (default 1.).
- Time period of the step (default 1.).
- Minimum time increment allowed. Only active if DIRECT is not specified. Default is the initial time increment or 1.e-5 times the time period of the step, whichever is smaller.
- Maximum time increment allowed. Only active if DIRECT is not specified. Default is 1.e+30.

Example:

```
*HEAT TRANSFER,DIRECT
.1,1.
```

defines a static step and selects the SPOOLES solver as linear equation solver in the step (default). The second line indicates that the initial time increment is .1 and the total step time is 1. Furthermore, the parameter DIRECT leads to a fixed time increment. Thus, if successful, the calculation consists of 10 increments of length 0.1.

Example files: beamhtcr, oneel20fi, oneel20rs.

Second line if FREQUENCY is selected:

- Number of eigenfrequencies desired.
- Lower value of requested eigenfrequency range (in cycles/time; default:0).

- Upper value of requested eigenfrequency range (in cycles/time; default: ∞).

```
Example:

*HEAT TRANSFER,FREQUENCY
8
```

defines a frequency step for the heat transfer equation. The eight lowest eigenvalues and corresponding eigenmodes are calculated. Notice that for the heat equation the following relation applies between the eigenvalue λ and eigenfrequency ω:

$$\lambda = -i\omega. \tag{339}$$

If, on the other hand, the heat transfer option is used as an alias for the Helmholtz equation, e.g. for acoustic problems, the same relationship as in elastodynamics

$$\lambda = \omega^2 \tag{340}$$

applies.

Second line if MODAL DYNAMIC is selected:

- Initial time increment. This value will be modified due to automatic incrementation, unless the parameter DIRECT was specified (default 1.).
- Time period of the step (default 1.).

Example files: aircolumn.

7.58 *HYPERELASTIC

Keyword type: model definition, material

This option is used to define the hyperelastic properties of a material. There are two optional parameters. The first one defines the model and can take one of the following strings: ARRUDA-BOYCE, MOONEY-RIVLIN, NEO HOOKE, OGDEN, POLYNOMIAL, REDUCED POLYNOMIAL or YEOH. The second parameter N makes sense for the OGDEN, POLYNOMIAL and REDUCED POLYMIAL model only, and determines the order of the strain energy potential. Default is the POLYNOMIAL model with N=1. All constants may be temperature dependent.

Let $\bar{I}_1$,$\bar{I}_2$ and J be defined by:

$$\bar{I}_1 = III_C^{-1/3} I_C \tag{341}$$

$$\bar{I}_2 = III_C^{-1/3} II_C \tag{342}$$

$$J = III_C^{1/2} \tag{343}$$

where I_C, II_C and III_C are the invariants of the right Cauchy-Green deformation tensor $C_{KL} = x_{k,K}x_{k,L}$. The tensor C_{KL} is linked to the Lagrange strain tensor E_{KL} by:

$$2E_{KL} = C_{KL} - \delta_{KL} \tag{344}$$

where δ is the Kronecker symbol.

The Arruda-Boyce strain energy potential takes the form:

$$\begin{aligned} U &= \mu\left\{\frac{1}{2}(\bar{I}_1 - 3) + \frac{1}{20\lambda_m^2}(\bar{I}_1^2 - 9) + \frac{11}{1050\lambda_m^4}(\bar{I}_1^3 - 27)\right. \\ &+ \left.\frac{19}{7000\lambda_m^6}(\bar{I}_1^4 - 81) + \frac{519}{673750\lambda_m^8}(\bar{I}_1^5 - 243)\right\} \\ &+ \frac{1}{D}\left(\frac{J^2-1}{2} - \ln J\right) \end{aligned} \tag{345}$$

The Mooney-Rivlin strain energy potential takes the form:

$$U = C_{10}(\bar{I}_1 - 3) + C_{01}(\bar{I}_2 - 3) + \frac{1}{D_1}(J-1)^2 \tag{346}$$

The Mooney-Rivlin strain energy potential is identical to the polynomial strain energy potential for $N = 1$.

The Neo-Hooke strain energy potential takes the form:

$$U = C_{10}(\bar{I}_1 - 3) + \frac{1}{D_1}(J-1)^2 \tag{347}$$

The Neo-Hooke strain energy potential is identical to the reduced polynomial strain energy potential for $N = 1$.

The polynomial strain energy potential takes the form:

$$U = \sum_{i+j=1}^{N} C_{ij}(\bar{I}_1 - 3)^i(\bar{I}_2 - 3)^j + \sum_{i=1}^{N}\frac{1}{D_i}(J-1)^{2i} \tag{348}$$

In CalculiX $N \leq 3$.

The reduced polynomial strain energy potential takes the form:

$$U = \sum_{i=1}^{N} C_{i0}(\bar{I}_1 - 3)^i + \sum_{i=1}^{N}\frac{1}{D_i}(J-1)^{2i} \tag{349}$$

In CalculiX $N \leq 3$. The reduced polynomial strain energy potential can be viewed as a special case of the polynomial strain energy potential

The Yeoh strain energy potential is nothing else but the reduced polynomial strain energy potential for $N = 3$.

Denoting the principal stretches by λ_1, λ_2 and λ_3 (λ_1^2, λ_2^2 and λ_3^2 are the eigenvalues of the right Cauchy-Green deformation tensor) and the deviatoric

stretches by $\bar{\lambda}_1$, $\bar{\lambda}_2$ and $\bar{\lambda}_3$, where $\bar{\lambda}_i = III_C^{-1/6}\lambda_i$, the Ogden strain energy potential takes the form:

$$U = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i^2}(\bar{\lambda}_1^{\alpha_i} + \bar{\lambda}_2^{\alpha_i} + \bar{\lambda}_3^{\alpha_i} - 3) + \sum_{i=1}^{N} \frac{1}{D_i}(J-1)^{2i}. \tag{350}$$

The input deck for a hyperelastic material looks as follows:

First line:

- *HYPERELASTIC
- Enter parameters and their values, if needed

Following line for the ARRUDA-BOYCE model:

- μ.
- λ_m.
- D.
- Temperature

Repeat this line if needed to define complete temperature dependence.
Following line for the MOONEY-RIVLIN model:

- C_{10}.
- C_{01}.
- D_1.
- Temperature

Repeat this line if needed to define complete temperature dependence.
Following line for the NEO HOOKE model:

- C_{10}.
- D_1.
- Temperature.

Repeat this line if needed to define complete temperature dependence.
Following line for the OGDEN model with N=1:

- μ_1.
- α_1.
- D_1.

- Temperature.

Repeat this line if needed to define complete temperature dependence.

Following line for the OGDEN model with N=2:

- μ_1.
- α_1.
- μ_2.
- α_2.
- D_1.
- D_2.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Following lines, in a pair, for the OGDEN model with N=3: First line of pair:

- μ_1.
- α_1.
- μ_2.
- α_2.
- μ_3.
- α_3.
- D_1.
- D_2.

Second line of pair:

- D_3.
- Temperature.

Repeat this pair if needed to define complete temperature dependence.

Following line for the POLYNOMIAL model with N=1:

- C_{10}.
- C_{01}.
- D_1.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Following line for the POLYNOMIAL model with N=2:

- C_{10}.
- C_{01}.
- C_{20}.
- C_{11}.
- C_{02}.
- D_1.
- D_2.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Following lines, in a pair, for the POLYNOMIAL model with N=3: First line of pair:

- C_{10}.
- C_{01}.
- C_{20}.
- C_{11}.
- C_{02}.
- C_{30}.
- C_{21}.
- C_{12}.

Second line of pair:

- C_{03}.
- D_1.
- D_2.
- D_3.
- Temperature.

Repeat this pair if needed to define complete temperature dependence.

Following line for the REDUCED POLYNOMIAL model with N=1:

- C_{10}.

- D_1.
- Temperature.

Repeat this line if needed to define complete temperature dependence.
Following line for the REDUCED POLYNOMIAL model with N=2:

- C_{10}.
- C_{20}.
- D_1.
- D_2.
- Temperature.

Repeat this line if needed to define complete temperature dependence.
Following line for the REDUCED POLYNOMIAL model with N=3:

- C_{10}.
- C_{20}.
- C_{30}.
- D_1.
- D_2.
- D_3.
- Temperature.

Repeat this line if needed to define complete temperature dependence.
Following line for the YEOH model:

- C_{10}.
- C_{20}.
- C_{30}.
- D_1.
- D_2.
- D_3.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

```
Example:

*HYPERELASTIC,OGDEN,N=1
3.488,2.163,0.
```

defines an ogden material with one term: $\mu_1 = 3.488$, $\alpha_1 = 2.163$, D_1=0. Since the compressibility coefficient was chosen to be zero, it will be replaced by CalculiX by a small value to ensure some compressibility to guarantee convergence (cfr. page 188).

Example files: beamnh, beamog.

7.59 *HYPERFOAM

Keyword type: model definition, material

This option is used to define a hyperfoam material. There is one optional parameters, N. N determines the order of the strain energy potential. Default is N=1. All constants may be temperature dependent.

The hyperfoam strain energy potential takes the form

$$U = \sum_{i=1}^{N} \frac{2\mu_i}{\alpha_i^2} \left[\lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3 + \frac{1}{\beta_i}(J^{-\alpha_i \beta_i} - 1) \right] \tag{351}$$

where λ_1, λ_2 and λ_3 are the principal stretches. The parameters β_i are related to the Poisson coefficients ν_i by:

$$\beta_i = \frac{\nu_i}{1 - 2\nu_i} \tag{352}$$

and

$$\nu_i = \frac{\beta_i}{1 + 2\beta_i}. \tag{353}$$

First line:

- *HYPERFOAM
- Enter parameters and their values, if needed

Following line for N=1:

- μ_1.
- α_1.
- ν_1.
- Temperature.

Repeat this line if needed to define complete temperature dependence.
Following line for N=2:

- μ_1.
- α_1.
- μ_2.
- α_2.
- ν_1.
- ν_2.
- Temperature.

Repeat this line if needed to define complete temperature dependence.
Following lines, in a pair, for N=3: First line of pair:

- μ_1.
- α_1.
- μ_2.
- α_2.
- μ_3.
- α_3.
- ν_1.
- ν_2.

Second line of pair:

- ν_3.
- Temperature.

Repeat this pair if needed to define complete temperature dependence.

`Example:`

```
*HYPERFOAM,N=2
0.164861,8.88413,2.302e-5,-4.81798,0.,0.
```

defines a hyperfoam material with two terms in the series.

Example files: beamhf.

7.60 *INCLUDE

Keyword type: step or model definition

The include statement allows to store part of the input deck in another file. There is only one required parameter, INPUT, taking the name of the file in or without double quotes ("). The double quotes are needed if the file name contains one or more blanks.

First line:

- *INCLUDE
- Enter the parameter and its value.

Example:

```
*INCLUDE,INPUT=/home/guido/test/beam.spc
```

is at execution time replaced by the contents of file /home/guido/test/beam.spc.

Example files: .

7.61 *INITIAL CONDITIONS

Keyword type: model definition

This option is used to define initial temperatures, initial velocities, initial stresses and initial plastic strains. There are two parameters: TYPE and USER. The parameter TYPE is required. It can take the following values:

- TYPE=DISPLACEMENT: initial displacements
- TYPE=FLUID VELOCITY: initial fluid velocities for 3D fluid calculations
- TYPE=MASS FLOW: initial mass flow for networks
- TYPE=PLASTIC STRAIN: initial inelastic strains
- TYPE=PRESSURE: initial static fluid pressures for 3D fluid calculations
- TYPE=SOLUTION: initial internal variables
- TYPE=STRESS: initial stresses
- TYPE=TEMPERATURE: initial temperatures for structural, network or 3D fluid calculations
- TYPE=TOTAL PRESSURE: initial total pressures for network calculations
- TYPE=VELOCITY: initial structural velocities (for dynamic calculations)

For shell elements TYPE=TEMPERATURE can be used to define an initial temperature gradient in addition to an initial temperature. The temperature applies to nodes in the reference surface, the gradient acts in normal direction. For beam elements two gradients can be defined: one in 1-direction and one in 2-direction. Default for the gradients is zero.

The plastic strain components defined with this option are subtracted from the strain components computed from the displacement field. If thermal strains are relevant they are additionally subtracted. The resulting strain is used to compute the stress and tangent stiffness matrix using the appropriate constitutive equations.

The parameter USER can only be used if TYPE=STRESS or TYPE=SOLUTION is specified. In that case, the user must define the initial stresses or internal variables by user routine sigini.f or sdvini.f, respectively.

Please note that vector and tensor quantities have to be provided in the GLOBAL (rectangular) coordinate system, no matter whether an *ORIENTATION card or *TRANSFORM card applies to the corresponding element or node, respectively.

First line:

- *INITIAL CONDITIONS
- Enter any needed parameters and their values.

Following line for TYPE=DISPLACEMENT:

- Node number or node set label.
- Degree of freedom in the GLOBAL coordinate system.
- Magnitude of the displacement.

Following line for TYPE=PLASTIC STRAIN:

- Element number.
- Integration point number.
- Value of first plastic strain component in the GLOBAL coordinate system.
- Value of second plastic strain component in the GLOBAL coordinate system.
- Etc.

Repeat this line if needed. The strain components should be given as Lagrange strain components for nonlinear calculations and linearized strain components for linear computations.

Following line for TYPE=PRESSURE, TYPE=TOTAL PRESSURE or TYPE=MASS FLOW:

- Node number or node set label.
- Static pressure, total pressure or mass flow value at the node.

Repeat this line if needed.

Following line for TYPE=SOLUTION if USER is not specified:

- Element number.
- Integration point number.
- Value of first internal variable.
- Value of second internal variable.
- Etc.

Repeat this line if needed. The number of internal variables must be specified by using the *DEPVAR card.

There is no line following the first one for TYPE=SOLUTION,USER.

Following line for TYPE=STRESS if USER is not specified:

- Element number.
- Integration point number.
- Value of first stress component in the GLOBAL coordinate system.
- Value of second stress component in the GLOBAL coordinate system.
- Etc.

Repeat this line if needed. The stress components should be given in the form of second Piola-Kirchhoff stresses.
There is no line following the first one for TYPE=STRESS,USER.

Following line for TYPE=TEMPERATURE:

- Node number or node set label.
- Initial temperature value at the node.
- Initial temperature gradient in normal direction (shells) or in 2-direction (beams).
- Initial temperature gradient in 1-direction (beams).

Repeat this line if needed.

Following line for TYPE=VELOCITY or TYPE=FLUID VELOCITY:

- Node number or node set label.
- Degree of freedom in the GLOBAL coordinate system.
- Magnitude of the velocity.

Examples:

```
*INITIAL CONDITIONS,TYPE=TEMPERATURE
Nall,273.
```

assigns the initial temperature T=273. to all nodes in (node) file Nall.

```
*INITIAL CONDITIONS,TYPE=VELOCITY
18,2,3.15
```

assigns the initial velocity 3.15 to degree of freedom 2 of node 18.

Example files: beam20t, beamnlt, beamt3, resstress1, resstress2, resstress3.

7.62 *MAGNETIC PERMEABILITY

Keyword type: model definition, material

This option is used to define the magnetic permeability of a material. There are no parameters. The material is supposed to be isotropic. The constant may be temperature dependent. The unit of the magnetic permeability coefficient is the unit of force divided by the square of the unit of electrical current. In SI-units this is N/A^2 or Henry/m. The magnetic permeability may be viewed as the product of the relative magnetic permeability (dimensionless) μ_r with the permeability of vacuum μ_0.

Following the magnetic permeability constant the user is supposed to define the domain for which this material is used. In an electromagnetic calculation there are three domains:

1. the air, which is the P-domain (domain 1)
2. the bodies, which is the A,V-domain (domain 2)
3. that part of the air, which, if filled with body material, ensures that the bodies are simply connected; this is the A-domain (domain 3). If there is only one body and if it is such that it is naturally simply connected the A-domain is empty.

For more details the reader is referred to the section on electromagnetism.

First line:

- *MAGNETIC PERMEABILITY

Following line:

- μ.
- number of the domain
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Example:

```
*MAGNETIC PERMEABILITY
1.255987E-6,2
```

tells you that the magnetic permeability coefficient is 1.255987×10^{-6}, independent of temperature (if SI-units are used this is the magnetic permeability of copper). The domain for which this material is defined is the A,V-domain.

Example files: induction.

7.63 *MATERIAL

Keyword type: model definition

This option is used to indicate the start of a material definition. A material data block is defined by the options between a *MATERIAL line and either another *MATERIAL line or a keyword line that does not define material properties. All material options within a data block will be assumed to define the same material. If a property is defined more than once for a material, the last definition is used. There is one required parameter, NAME, defining the name of the material with which it can be referenced in element property options (e.g. *SOLID SECTION). The name can contain up to 80 characters.

Material data requests outside the defined ranges are extrapolated in a constant way and a warning is generated. Be aware that this occasionally occurs due to rounding errors.

First line:

- *MATERIAL
- Enter the NAME parameter and its value.

Example:

```
*MATERIAL,NAME=EL
```

starts a material block with name EL.

Example files: fullseg, beamnldype, beamog.

7.64 *MODAL DAMPING

Keyword type: step

This card is used within a step in which the *MODAL DYNAMIC or *STEADY STATE DYNAMICS procedure has been selected. There are two optional, mutually exclusive parameters: RAYLEIGH and MODAL=DIRECT (default).

If MODAL=DIRECT is selected the user can specify the viscous damping factor ζ for each mode separately. This is the default. Direct damping is not allowed in combination with nonzero single point constraints.

If RAYLEIGH is selected Rayleigh damping is applied in a global way, i.e. the damping matrix $[C]$ is taken to be a linear combination of the stiffness matrix $[K]$ and the mass matrix $[M]$:

$$[C] = \alpha [M] + \beta [K] . \tag{354}$$

The coefficients apply to all modes. The corresponding viscous damping factor ζ_j for mode j amounts to:

$$\zeta_j = \frac{\alpha}{2\omega_j} + \frac{\beta\omega_j}{2}. \tag{355}$$

Consequently, α damps the low frequencies, β damps the high frequencies.

The *MODAL DAMPING keyword can be used in any step to redefine damping values defined in a previous step.

First line:

- *MODAL DAMPING,RAYLEIGH
- Enter any needed parameters and their values.

Second line if MODAL=DIRECT is selected (or, since this is default, if no additional parameter is entered):

- lowest mode of the range
- highest mode of the range (default is lowest mode of the range)
- viscous damping factor ζ for modes between (and including) the lowest and highest mode of the range

Repeat this line if needed.

Second line if RAYLEIGH is selected:

- not used (kept for compatibility reasons with ABAQUS)
- not used (kept for compatibility reasons with ABAQUS)
- Coefficient of the mass matrix α.
- Coefficient of the stiffness matrix β.

```
Example:

*MODAL DAMPING,RAYLEIGH
,,0.,2.e-4
```

indicates that the damping matrix is obtained by multiplying the stiffness matrix with $2 \cdot 10^{-4}$

Example files: beamdy3, beamdy4, beamdy5, beamdy6.

7.65 *MODAL DYNAMIC

Keyword type: step

This procedure is used to calculate the response of a structure subject to dynamic loading. Although the deformation up to the onset of the dynamic calculation can be nonlinear, this procedure is basically linear and assumes that the response can be written as a linear combination of the lowest modes of the structure. To this end, these modes must have been calculated in a previous *FREQUENCY,STORAGE=YES step (not necessarily in the same calculation). In the *MODAL DYNAMIC step the eigenfrequencies, modes and mass matrix are recovered from the file jobname.eig. The time period of the loading is characterized by its total length and the length of an increment. Within each increment the loading is assumed to be linear, in which case the solution is exact apart from modeling inaccuracies and the fact that not all eigenmodes are used. The number of eigenmodes used is taken from the previous *FREQUENCY step. Since a modal dynamic step is a perturbation step, all previous loading is removed. The loading defined within the step is multiplied by the amplitude history for each load as specified by the AMPLITUDE parameter on the loading card, if any. If no amplitude applies all loading is applied at the start of the step. Loading histories extending beyond the amplitude time scale are extrapolated in a constant way. The absence of the AMPLITUDE parameter on a loading card leads to a constant load.

There are four optional parameters: SOLVER, DIRECT, DELTMX, and STEADY STATE. SOLVER determines the package used to solve for the steady state solution in the presence of nonzero displacement boundary conditions. The following solvers can be selected:

- the SGI solver
- PARDISO
- SPOOLES [3, 4].
- TAUCS

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, an error is issued.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU decomposition, however, I was not able to run either of them so far. PARDISO is the Intel proprietary solver.

The parameters DIRECT and DELTMX are linked. The parameter DIRECT controls the increment size. If DIRECT=NO the size of increments is variable. It is determined by the requirement that the change in forces within an increment should not exceed the value of DELTMX. Therefore, if the user specifies DIRECT=NO a value for DELTMX has to be provided. Default is DIRECT=YES (or, equivalently DIRECT without any argument). In the latter case the value of DELTMX is irrelevant. The modal forces are the scalar product of the system force vector with each of the selected (mass normalized) eigenmodes. The unit of the modal forces is force times square root of length.

The parameter STEADY STATE can be used to continue a modal dynamics calculation until steady state has been reached. In that case the total time period is set to $10.^{10}$ and does not have to be specified by the user. Instead, the user defines the maximum allowable relative error for the solution to be considered to be steady state. For instance, if the user sets this number to 0.01 steady state will be reached if the change in the largest solution variable (displacements or temperatures, depending on the kind of analysis) does not exceed 1%.

First line:

- *MODAL DYNAMIC
- enter the SOLVER parameter and its value, if needed.

Second line if STEADY STATE is not active:

- Initial time increment. This value will be modified due to automatic incrementation, if DIRECT=NO was specified. If no value is given, the initial time increment equals the time period of the step.
- Time period of the step.
- Minimum time increment allowed. Only active if DIRECT=NO is specified. Default is the initial time increment or 1.e-10 times the time period of the step, whichever is smaller.
- Maximum time increment allowed. Only active if DIRECT=NO is specified. Default is 1.e+30.

Second line if STEADY STATE is active:

- Initial time increment. This value will be modified due to automatic incrementation if DIRECT=NO was specified.
- Relative error for steady state conditions to be satisfied.
- Minimum time increment allowed. Only active if DIRECT=NO is specified. Default is the initial time increment or 1.e-10 times the time period of the step, whichever is smaller.
- Maximum time increment allowed. Only active if DIRECT=NO is specified. Default is 1.e+30.

```
Example:

*MODAL DYNAMIC
1.E-5,1.E-4
```

defines a modal dynamic procedure with time increment 10^{-5} and time period 10^{-4}. The time increment is kept constant.

```
Example:

*MODAL DYNAMIC,STEADY STATE
1.E-5,1.E-2
```

defines a modal dynamic procedure with initial time increment 10^{-5} and relative error 10^{-2}. The time increment is kept constant.

Example files: beamdy1, beamdy2, beamdy3, beamdy4, beamdy5, beamdy6, beamdy17.

7.66 *MODEL CHANGE

Keyword type: step

With this option one can activate or deactivate elements and contact pairs.

One can deactivate or activate any element which has been defined in the model section of the input deck. Before the first step all elements are by default activated. There is one required parameter TYPE=ELEMENT and there are two mutually exclusive parameters ADD and REMOVE.

To activate or deactivate contact between two surfaces, contact must have been defined between these surfaces using a *CONTACT PAIR card before the first step. By default all contact pairs are activated before the first step. There is one required parameter TYPE=CONTACT PAIR and there are two mutually exclusive parameters ADD and REMOVE.

First line:

- *MODEL CHANGE

- enter the required parameter TYPE=CONTACT PAIR or TYPE=ELEMENT and one of the mutually exclusive parameters ADD and REMOVE.

Following line for TYPE=ELEMENT:

- List of elements and/or sets of elements to be activated or deactivated (maximum 16 entries per line).

Repeat this line if needed

Following line for TYPE=CONTACT PAIR:

- Name of the slave surface (can be nodal or element face based).

- Name of the master surface (must be based on element faces).

Example:

```
*MODEL CHANGE,TYPE=CONTACT PAIR,REMOVE
dep,ind
```

deactivates contact between the surfaces dep and ind.

Example files: modelchel

7.67 *MPC

Keyword type: model definition

With this keyword card a multiple point constraint is defined, usually a nonlinear one. Right now, three different MPC's can be selected.

- A plane MPC (name PLANE). This MPC specifies that all nodes listed within this MPC card should stay in a plane. The first three nodes are the defining nodes and should not lie on a line. For all subsequent nodes a nonlinear MPC is generated expressing that they stay within the plane. Notice that the plane can move during deformation, depending on the motion of the defining nodes.

- A straight line MPC (name STRAIGHT). This MPC expresses that all nodes listed within this MPC card should stay on a straight line. The first two nodes are the defining nodes and should not coincide. For all subsequent nodes two nonlinear MPC's are generated expressing that they stay on the straight line. Notice that the straight line can move during deformation, depending on the motion of its defining nodes.

- A user MPC (name to be defined by the user). With this option the user can define new nonlinear MPC's.

A *MPC card automatically triggers the NLGEOM parameter, i.e. a geometrically nonlinear calculation is performed, except if the MPC is a mean rotation MPC.

There are no parameters for this keyword card.

First line:

- *MPC

Second line:

- MPC name
- list of nodes participating in the MPC: maximum 15 entries. Zero entries are discarded.

Following lines (as many as needed):

- list of nodes participating in the MPC: maximum 16 entries. Zero entries are discarded.

Example:

```
*MPC
PLANE,3,8,15,39,14
```

specifies that nodes 3, 8, 15, 39 and 14 should stay in a plane. The plane is defined by nodes 3, 8 and 15. They should not be co-linear.

Example files: beammr, beamplane, beamstraight.

7.68 *NO ANALYSIS

Keyword type: step

This procedure is used for input deck and geometry checking only. No calculation is performed. There are no parameters.

First and only line:

- *NO ANALYSIS

Example:

```
*NO ANALYSIS
```

requests the no analysis procedure, in which the set of equations is built but not solved (the Jacobian determinant is checked).

Example files: beamnoan.

7.69 *NODAL THICKNESS

Keyword type: model definition

This option is used to assign a thickness to a node or to a node set. There are no parameters. This keyword only makes sense for nodes belonging to plane stress elements, shell elements and beam elements. For all of these except for the beam elements one thickness value should be given. For plane stress and shell elements this is the thickness in normal direction. The normal direction can be defined by using the *NORMAL keyword card. If none is defined, the normal is calculated based on the geometrical data. For beam elements two thicknesses can be defined: one in 1-direction and one in 2-direction. The 1-direction can be defined on the *BEAM SECTION card, the 2-direction by the *NORMAL card.

The *NODAL THICKNESS card takes precedence over any thickness definitions on the *BEAM SECTION or *SHELL SECTION card. Right now, it cannot be used for composite materials.

First line:

- *NODAL THICKNESS

Following line:

- Node or set of nodes previously defined
- Thickness 1
- Thickness 2

Example:

```
*NODAL THICKNESS
22,0.05,0.08
```

assigns to node 22 the thickness 0.05 and 0.08. Any plane stress or shell element containing node 22 will have a local thickness of 0.05 unit lengths at node 22. Any beam element containing node 22 will have a thickness of 0.05 unit length in local 1-direction and a thickness of 0.08 unit length in local 2-direction.

Example files: shell1.

7.70 *NODE

Keyword type: model definition

This option allows nodes and their coordinates to be defined. The parameter NSET is optional and is used to assign the nodes to a node set. If the set already exists, the nodes are ADDED to the set.

First line:

- *NODE
- Enter the optional parameter, if desired.

Following line:

- node number.
- Value of first coordinate.
- Value of second coordinate.
- Value of third coordinate.

Repeat this line if needed.

Example:

```
*NODE,NSET=Nall
1,0.,0.,0.
2,1.,0.,0.
3,0.,1.,0.
```

defines three nodes with node number one, two and three and rectangular coordinates (0.,0.,0.), (1.,0.,0.) and (0.,1.,0.) respectively.

Example files: beam8t, beamb, beamdy1.

7.71 *NODE FILE

Keyword type: step

This option is used to print selected nodal variables in file jobname.frd for subsequent viewing by CalculiX GraphiX. The following variables can be selected (the label is square brackets [] is the one used in the .frd file; for frequency calculations with cyclic symmetry both a real and an imaginary part may be stored, in all other cases only the real part is stored):

- CP: Pressure coefficient in 3D compressible fluids.
- DEPT [DEPTH]: Fluid depth in channel networks.
- HCRI [HCRIT]: Critical depth in channel networks.
- MACH: Mach numbers in 3D compressible fluids.
- MAXU [MDISP]: Maximum displacements orthogonal to a given vector at all times for *FREQUENCY calculations with cyclic symmetry. The components of the vector are the coordinates of a node stored in a node set with the name RAY. This node and node set must have been defined by the user.

- MF [MAFLOW]: Mass flows in networks. The mass flow through a network element is stored in the middle node of the element. In the end nodes the mass flow is not unique, since more than two element can be connected to the node. For end nodes the sum of the mass flow leaving the node is stored. Notice that at nodes where mass flow is leaving the network the value will be wrong if no proper exit element (with node number 0) is attached to that node.
- NT [NDTEMP]: Temperatures. This includes both structural temperatures and total fluid temperatures in a network.
- PNT [PNDTEMP]: Temperatures: magnitude and phase (only for *STEADY STATE DYNAMICS calculations).
- POT [ELPOT]: Electrical potential, only for electromagnetic calculations.
- PRF [PFORC]: External forces: magnitude and phase (only for *FREQUENCY calculations with cyclic symmetry).
- PS [STPRES]: Static pressures in liquid networks.
- PSF: Static pressures in 3D fluids.
- PT [TOPRES]: Total pressures in gas networks.
- PTF: Total pressures in 3D fluids.
- PU [PDISP]: Displacements: magnitude and phase (only for *STEADY STATE DYNAMICS calculations and *FREQUENCY calculations with cyclic symmetry).
- RF [FORC(real), FORCI(imaginary)]: External forces (only static forces; dynamic forces, such as those caused by dashpots, are not included)
- RFL [RFL]: External concentrated heat sources.
- TS [STTEMP]: Static temperatures in networks.
- TSF: Static temperatures in 3D fluids.
- TT [TOTEMP]: Total temperatures in networks.
- TTF: Total temperatures in 3D fluids.
- TURB: Turbulence variables in 3D compressible fluids: ρk and $\rho\omega$.
- U [DISP(real), DISPI(imaginary)]: Displacements.
- V [VELO]: Velocities in dynamic calculations.
- VF: Velocities in 3D fluids.

The selected variables are stored for the complete model.

The external forces (key RF) are the sum of the reaction forces, concentrated loads (*CLOAD) and distributed loads (*DLOAD) in the node at stake. Only in the absence of concentrated loads in the node and distributed loads in any element to which the node belongs, the external forces reduce to the reaction forces. Forces induced by multiple point constraints are not calculated. Since single point constraints defined in transformed coordinates are converted into multiple point constraints in the global rectangular system, the force in a node in which a SPC is defined in local coordinates are not correctly delivered upon using the RF key in combination with the *NODE PRINT keyword card.

For frequency calculations with cyclic symmetry the eigenmodes are generated in pairs (different by a phase shift of 90 degrees). Only the first one of each pair is stored in the frd file. If U is selected (the displacements) two load cases are stored in the frd file: a loadcase labeled DISP containing the real part of the displacements and a loadcase labeled DISPI containing the imaginary part of the displacements. For all other variables only the real part is stored.

The first occurrence of an *NODE FILE keyword card within a step wipes out all previous nodal variable selections for file output. If no *NODE FILE card is used within a step the selections of the previous step apply. If there is no previous step, no nodal variables will be stored.

Notice that only values in nodes belonging to elements are stored. Values in nodes not belonging to any element (e.g. the rotational node in a *RIGID BODY option) can only be obtained using *NODE PRINT.

There are seven optional parameters: FREQUENCY, FREQUENCYF, GLOBAL, OUTPUT, TIME POINTS, NSET, LAST ITERATIONS and CONTACT ELEMENTS. The parameters FREQUENCY and TIME POINTS are mutually exclusive.

FREQUENCY applies to nonlinear calculations where a step can consist of several increments. Default is FREQUENCY=1, which indicates that the results of all increments will be stored. FREQUENCY=N with N an integer indicates that the results of every Nth increment will be stored. The final results of a step are always stored. If you only want the final results, choose N very big. The value of N applies to *OUTPUT,*ELEMENT OUTPUT, *EL FILE, *ELPRINT, *NODE OUTPUT, *NODE FILE, *NODE PRINT, *FACE PRINT,*CONTACT OUTPUT *CONTACT FILE and *CONTACT PRINT. If the FREQUENCY parameter is used for more than one of these keywords with conflicting values of N, the last value applies to all. A frequency parameter stays active across several steps until it is overwritten by another FREQUENCY value or the TIME POINTS parameter.

The 3D fluid analogue of FREQUENCY is FREQUENCYF. In coupled calculations FREQUENCY applies to the thermomechanical output, FREQUENCYF to the 3D fluid output.

With the parameter GLOBAL you tell the program whether you would like the results in the global rectangular coordinate system or in the local nodal system. If an *TRANSFORM card is applied to the node at stake, this card defines the local system. If no *TRANSFORM card is applied to the element,

the local system coincides with the global rectangular system. Default value for the GLOBAL parameter is GLOBAL=YES, which means that the results are stored in the global system. If you prefer the results in the local system, specify GLOBAL=NO.

The parameter OUTPUT can take the value 2D or 3D. This has only effect for 1d and 2d elements such as beams, shells, plane stress, plane strain and axisymmetric elements AND provided it is used in the first step. If OUTPUT=3D, the 1d and 2d elements are stored in their expanded three-dimensional form. In particular, the user has the advantage to see his/her 1d/2d elements with their real thickness dimensions. However, the node numbers are new and do not relate to the node numbers in the input deck. Once selected, this parameter is active in the complete calculation. If OUTPUT=2D the fields in the expanded elements are averaged to obtain the values in the nodes of the original 1d and 2d elements. In particular, averaging removes the bending stresses in beams and shells. Therefore, default for beams and shells is OUTPUT=3D, for plane stress, plane strain and axisymmetric elements it is OUTPUT=2D. For axisymmetric structures and OUTPUT=2D the mass flow (MF) and the external force (RF) are stored for 360°, else it is stored for the displayed 3D segment, i.e. 2°.

With the parameter TIME POINTS a time point sequence can be referenced, defined by a *TIME POINTS keyword. In that case, output will be provided for all time points of the sequence within the step and additionally at the end of the step. No other output will be stored and the FREQUENCY parameter is not taken into account. Within a step only one time point sequence can be active. If more than one is specified, the last one defined on any of the keyword cards *NODE FILE, *EL FILE, *NODE PRINT or *EL PRINT will be active. The TIME POINTS option should not be used together with the DIRECT option on the procedure card. The TIME POINTS parameters stays active across several steps until it is replaced by another TIME POINTS value or the FREQUENCY parameter.

The specification of a node set with the parameter NSET limits the output to the nodes contained in the set. For cyclic symmetric structures the usage of the parameter NGRAPH on the *CYCLIC SYMMETRY MODEL card leads to output of the results not only for the node set specified by the user (which naturally belongs to the base sector) but also for all corresponding nodes of the sectors generated by the NGRAPH parameter. Notice that for cyclic symmetric structures the use of NSET is mandatory.

The parameter LAST ITERATIONS leads to the storage of the displacements in all iterations of the last increment in a file with name ResultsForLastIterations.frd (can be opened with CalculiX GraphiX). This is useful for debugging purposes in case of divergence. No such file is created if this parameter is absent.

Finally, the parameter CONTACT ELEMENTS stores the contact elements which have been generated in each iteration in a file with the name contactelements.inp. When opening the frd file with CalculiX GraphiX these files can be read with the command "read contactelements.inp" and visualized by plotting the elements in the sets contactelements_stα_inβ_atγ_itδ, where α is the step

number, β the increment number, γ the attempt number and δ the iteration number.

First line:

- *NODE FILE
- Enter any needed parameters and their values.

Second line:

- Identifying keys for the variables to be printed, separated by commas.

Example:

```
*NODE FILE,TIME POINTS=T1
RF,NT
```

requests the storage of reaction forces and temperatures in the .frd file for all time points defined by the T1 time points sequence.

Example files: beampt, beampo1.

7.72 *NODE OUTPUT

Keyword type: step

This option is used to print selected nodal variables in file jobname.frd for subsequent viewing by CalculiX GraphiX. The options and its use are identical with the *NODE FILE keyword, however, the resulting .frd file is a mixture of binary and ASCII (the .frd file generated by using *NODE FILE is completely ASCII). This has the advantage that the file is smaller and can be faster read by cgx.

Example:

```
*NODE OUTPUT,FREQUENCY=2,TIME POINTS=T1
RF,NT
```

requests the storage of reaction forces and temperatures in the .frd file every second increment. In addition, output will be stored for all time points defined by the T1 time points sequence.

Example files: cubespring.

7.73 *NODE PRINT

Keyword type: step

This option is used to print selected nodal variables in file jobname.dat. The following variables can be selected:

- Displacements (key=U)
- Structural temperatures and total temperatures in networks (key=NT or TS; both are equivalent)
- Static temperatures in 3D fluids (key=TSF)
- Total temperatures in 3D fluids (key=TTF)
- Pressures in networks (key=PN). These are the total pressures for gases, static pressures for liquids and liquid depth for channels. The fluid section types dictate the kind of network.
- Static pressures in 3D fluids (key=PSF)
- Total pressures in 3D fluids (key=PTF)
- Mach numbers in compressible 3D fluids (key=MACH)
- Pressure coefficients in compressible 3D fluids (key=CP)
- Velocities in 3D fluids (key=VF)
- Mass flows in networks (key=MF)
- External forces (key=RF) (only static forces; dynamic forces, such as those caused by dashpots, are not included)
- External concentrated heat sources (key=RFL)

The external forces are the sum of the reaction forces, concentrated loads (*CLOAD) and distributed loads (*DLOAD) in the node at stake. Only in the absence of concentrated loads in the node and distributed loads in any element to which the node belongs, the external forces reduce to the reaction forces. Forces induced by multiple point constraints are not calculated. Since single point constraints defined in transformed coordinates are converted into multiple point constraints in the global rectangular system, the force in a node in which a SPC is defined in local coordinates are not correctly delivered upon using the RF key in combination with the *NODE PRINT keyword card.

There are six parameters, FREQUENCY, FREQUENCYF, NSET, TOTALS, GLOBAL and TIME POINTS. The parameter NSET is required, defining the set of nodes for which the displacements should be printed. If this card is omitted, no values are printed. Several *NODE PRINT cards can be used within one and the same step.

The parameters FREQUENCY and TIME POINTS are mutually exclusive.

The parameter FREQUENCY is optional, and applies to nonlinear calculations where a step can consist of several increments. Default is FREQUENCY=1, which indicates that the results of all increments will be stored. FREQUENCY=N with N an integer indicates that the results of every Nth increment will be stored. The final results of a step are always stored. If you only want the final results, choose N very big. The value of N applies to *OUTPUT,*ELEMENT OUTPUT, *EL FILE, *ELPRINT, *NODE OUTPUT, *NODE FILE, *NODE PRINT, *FACE PRINT,*CONTACT OUTPUT, *CONTACT FILE and *CONTACT PRINT. If the FREQUENCY parameter is used for more than one of these keywords with conflicting values of N, the last value applies to all. A frequency parameter stays active across several steps until it is overwritten by another FREQUENCY value or the TIME POINTS parameter.

The 3D fluid analogue of FREQUENCY is FREQUENCYF. In coupled calculations FREQUENCY applies to the thermomechanical output, FREQUENCYF to the 3D fluid output.

The parameter TOTALS only applies to external forces. If TOTALS=YES the sum of the external forces for the whole node set is printed in addition to their value for each node in the set separately. If TOTALS=ONLY is selected the sum is printed but the individual nodal contributions are not. If TOTALS=NO (default) the individual contributions are printed, but their sum is not. Notice that the sum is always written in the global rectangular system, irrespective of the value of the GLOBAL parameter.

With the optional parameter GLOBAL you tell the program whether you would like the results in the global rectangular coordinate system or in the local nodal system. If an *TRANSFORM card is applied to the node at stake, this card defines the local system. If no *TRANSFORM card is applied to the element, the local system coincides with the global rectangular system. Default value for the GLOBAL parameter is GLOBAL=NO, which means that the results are stored in the local system. If you prefer the results in the global system, specify GLOBAL=YES.

With the parameter TIME POINTS a time point sequence can be referenced, defined by a *TIME POINTS keyword. In that case, output will be provided for all time points of the sequence within the step and additionally at the end of the step. No other output will be stored and the FREQUENCY parameter is not taken into account. Within a step only one time point sequence can be active. If more than one is specified, the last one defined on any of the keyword cards *NODE FILE, *EL FILE, *NODE PRINT, *EL PRINT or *FACE PRINT will be active. The TIME POINTS option should not be used together with the DIRECT option on the procedure card. The TIME POINTS parameters stays active across several steps until it is replaced by another TIME POINTS value or the FREQUENCY parameter.

The first occurrence of an *NODE PRINT keyword card within a step wipes out all previous nodal variable selections for print output. If no *NODE PRINT card is used within a step the selections of the previous step apply, if any.

Notice that some of the keys apply to specific domains. For instance, PS and V can only be used for 3D fluids, PT and MF only for networks. Furthermore,

PT only makes sense for the vertex nodes of the network elements, whereas MF only applies to the middle nodes of network elements. It is the responsibility of the user to make sure that the sets (s)he specifies contain the right nodes. For nodes not matching the key the printed values are meaningless. If the model contains axisymmetric elements the mass flow applies to a segment of 2°. So for the total flow this value has to be multiplied by 180.

First line:

- *NODE PRINT
- Enter the parameter NSET and its value.

Second line:

- Identifying keys for the variables to be printed, separated by commas.

```
Example:

*NODE PRINT,NSET=N1
RF
```

requests the storage of the reaction forces in the nodes belonging to (node) set N1 in the .dat file.

Example files: beampkin, beamrb.

7.74 *NORMAL

Keyword type: model definition

With this option a normal can be defined for a (node,element) pair. This only makes sense for shell elements and beam elements. For beam elements the normal direction is the local 2-direction. If no normal is specified in a node it is calculated on basis of the local geometry. If the normal defined by the user has not unit length, it will be normalized. There are no parameters for this keyword card.

First line:

- *NORMAL
- Element number
- Node number
- Global x-coordinate of the normal
- Global y-coordinate of the normal
- Global z-coordinate of the normal

Example:

```
*NORMAL
5,18,0.707,0.,0.707
```

Defines a normal with components (0.707,0.,0.707) in node 18 of element 5.

Example files: shellnor.

7.75 *NSET

Keyword type: model definition

This option is used to assign nodes to a node set. The parameter NSET containing the name of the set is required (maximum 80 characters), whereas the parameter GENERATE (without value) is optional. If present, nodal ranges can be expressed by their initial value, their final value, and an increment. If a set with the same name already exists, it is reopened and complemented. The name of a set is case insensitive. Internally, it is modified into upper case and a 'N' is appended to denote it as node set. Nodes are internally stored in the order they are entered, no sorting is performed.

First line:

- *NSET
- Enter any needed parameters and their values.

Following line if the GENERATE parameter is omitted:

- List of nodes and/or sets of nodes previously defined to be assigned to this node set (maximum 16 entries per line).

Repeat this line if needed.

Following line if the GENERATE parameter is included:

- First node in set.
- Last node in set.
- Increment in nodal numbers between nodes in the set. Default is 1.

Repeat this line if needed.

Example:

```
*NSET,NSET=N1
1,8,831,208
*NSET,NSET=N2
100,N1
```

assigns the nodes with number 1, 8, 831 and 208 to (node) set N1 and the nodes with numbers 1, 8, 831, 208 (= set N1) and 100 to set N2.

Example files: segmentm, shell2.

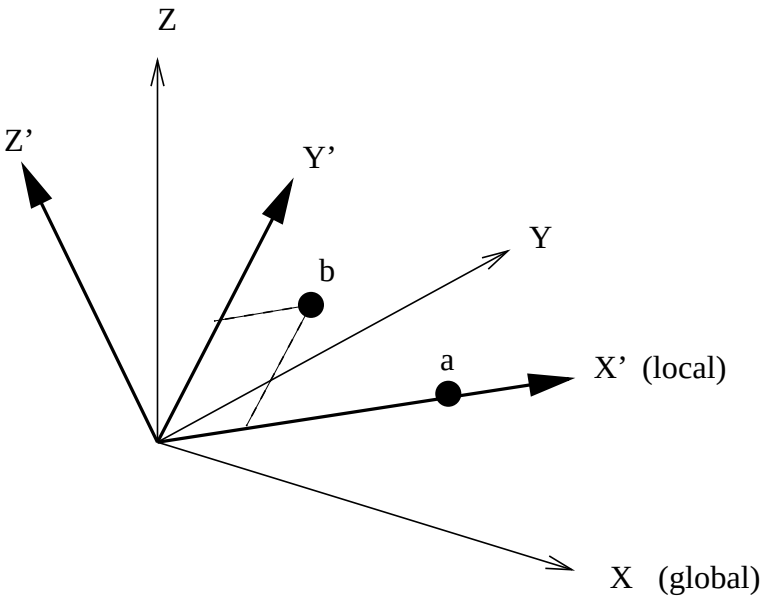


Figure 130: Definition of a rectangular coordinate system

7.76 *ORIENTATION

Keyword type: model definition

This option may be used to specify a local axis system X'-Y'-Z' to be used for defining material properties. For now, rectangular and cylindrical systems can be defined, triggered by the parameter SYSTEM=RECTANGULAR (default) and SYSTEM=CYLINDRICAL.

A rectangular system is defined by specifying a point a on the local X' axis and a point b belonging to the X'-Y' plane but not on the X' axis. A right hand system is assumed (Figure 130).

When using a cylindrical system two points a and b on the axis must be given. The X' axis is in radial direction, the Z' axis in axial direction from point a to point b, and Y' is in tangential direction such that X'-Y'-Z' is a right hand system (Figure 131).

The parameter NAME, specifying a name for the orientation so that it can be used in an element property definition (e.g. *SOLID SECTION) is required (maximum 80 characters).

First line:

- *ORIENTATION
- Enter the required parameter NAME, and the optional parameter SYSTEM if needed.

Second line:

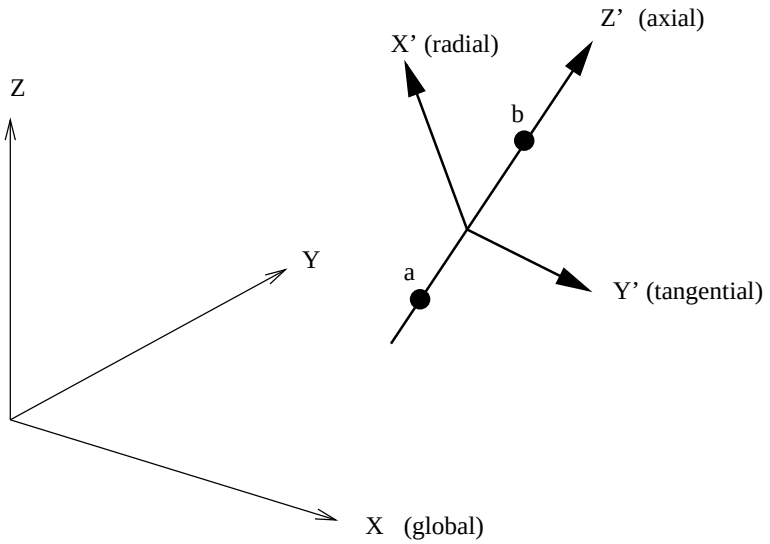


Figure 131: Definition of a cylindrical coordinate system

- X-coordinate of point a.
- Y-coordinate of point a.
- Z-coordinate of point a.
- X-coordinate of point b.
- Y-coordinate of point b.
- Z-coordinate of point b.

```
Example:

*ORIENTATION,NAME=OR1,SYSTEM=CYLINDRICAL
0.,0.,0.,1.,0.,0.
```

defines a cylindrical coordinate system with name OR1 and axis through the points (0.,0.,0.) and (1.,0.,0.). Thus, the x-axis in the global coordinate system is the axial direction in the cylindrical system.

Example files: beampo2.

7.77 *OUTPUT

Keyword type: model definition

This keyword is provided for compatibility with ABAQUS. The only parameters are FREQUENCY and FREQUENCYF. They are optional.

The parameter FREQUENCY applies to nonlinear calculations where a step can consist of several increments. Default is FREQUENCY=1, which indicates that the results of all increments will be stored. FREQUENCY=N with N an integer indicates that the results of every Nth increment will be stored. The final results of a step are always stored. If you only want the final results, choose N very big. The value of N applies to *OUTPUT,*ELEMENT OUTPUT, *EL FILE, *ELPRINT, *NODE OUTPUT, *NODE FILE, *NODE PRINT, *FACE PRINT,*CONTACT OUTPUT *CONTACT FILE and *CONTACT PRINT. If the FREQUENCY parameter is used for more than one of these keywords with conflicting values of N, the last value applies to all. A frequency parameter stays active across several steps until it is overwritten by another FREQUENCY value or the TIME POINTS parameter.

The 3D fluid analogue of FREQUENCY is FREQUENCYF. In coupled calculations FREQUENCY applies to the thermomechanical output, FREQUENCYF to the 3D fluid output.

7.78 *PHYSICAL CONSTANTS

Keyword type: model definition

This keyword is used to define the Stefan–Boltzmann constant, absolute zero temperature and the universal gravitational constant in the user's units. For 3D fluid calculations only absolute zero temperature is needed, for radiation type boundary conditions both absolute zero temperature and the Stefan–Boltzmann constant must be defined. They are defined by the two parameters ABSOLUTE ZERO and STEFAN BOLTZMANN. The universal gravitational constant is required for general gravitational loading, e.g. for the calculation of orbits and is defined by the parameter NEWTON GRAVITATION.

First line:

- *PHYSICAL CONSTANTS

Example:

```
*PHYSICAL CONSTANTS, ABSOLUTE ZERO=0, STEFAN BOLTZMANN=5.669E-8
```

for time in s, length in m, mass in kg and temperature in K (unit of the Stefan-Boltzmann constant: $Wm^{-2}K^{-4}$.

Example:

```
*PHYSICAL CONSTANTS, NEWTON GRAVITY=6.67E-11
```

for time in s, length in m, mass in kg and temperature in K (unit of the universal gravitational constant: Nm^2kg^{-2}).

Example files: beamhtbf, oneel20cf, cubenewt.

7.79 *PLASTIC

Keyword type: model definition, material

This option is used to define the plastic properties of an incrementally plastic material. There is one optional parameter HARDENING. Default is HARDENING=ISOTROPIC, other values are HARDENING=KINEMATIC for kinematic hardening, HARDENING=COMBINED for combined isotropic and kinematic hardening and HARDENING=USER for user defined hardening curves. All constants may be temperature dependent. The card should be preceded by a *ELASTIC card within the same material definition, defining the isotropic elastic properties of the material. User defined hardening curves should be defined in the user subroutine uhardening.f

If the elastic data is isotropic, the large strain viscoplastic theory treated in [68] and [69] is applied. If the elastic data is orthotropic, the infinitesimal strain model discussed in Section 6.8.11 is used. Accordingly, for an elastically orthotropic material the hardening can be at most linear. Furthermore, if the temperature data points for the hardening curves do not correspond to the *ELASTIC temperature data points, they are interpolated at the latter points. Accordingly, for an elastically orthotropic material, it is advisable to define the hardening curves at the same temperatures as the elastic data.

For the selection of plastic output variables the reader is referred to Section 6.8.6.

First line:

- *PLASTIC
- Enter the HARDENING parameter and its value, if needed

Following sets of lines define the isotropic hardening curve for HARDENING=ISOTROPIC and the kinematic hardening curve for HARDENING=KINEMATIC or HARDENING=COMBINED: First line in the first set:

- Von Mises stress.
- Equivalent plastic strain.
- Temperature.

Use as many lines in the first set as needed to define the complete hardening curve for this temperature.

Use as many sets as needed to define complete temperature dependence.

For the definition of the isotropic hardening curve for HARDENING=COMBINED the keyword *CYCLIC HARDENING is used.

Example:

```
*PLASTIC
800.,0.,273.
```

```
900.,0.05,273.
1000.,0.15,273.
700.,0.,873.
750.,0.04,873.
800.,0.13,873.
```

defines two stress-strain curves: one for temperature T=273. and one for T=873. The curve at T=273 connects the points (800.,0.), (900.,0.05) and (1000.,0.15), the curve at T=873 connects (700.,0.), (750.,0.04) and (800.,0.13). Notice that the first point on the curves represents first yielding and must give the Von Mises stress for a zero equivalent plastic strain.

Example files: beampd, beampiso, beampkin, beampt.

7.80 *PRE-TENSION SECTION

Keyword type: model definition

This option is used to define a pre-tension in a bolt or similar structure. There are three parameters: SURFACE, ELEMENT and NODE. The parameter NODE is required as well as one of the parameters SURFACE and ELEMENT. The latter two parameters are mutually exclusive.

With the parameter SURFACE an element face surface can be defined on which the pre-tension acts. This is usually a cross section of the bolt. This option is used for volumetric elements. Alternatively, the bolt can be modeled with just one linear beam element (type B31). In that case the parameter ELEMENT is required pointing to the label of the beam element.

The parameter NODE is used to define a reference node. This node should not be used elsewhere in the model. In particular, it should not belong to any element. The coordinates of this node are immaterial. The first degree of freedom of this node is used to define a pre-tension force with *CLOAD or a differential displacement with *BOUNDARY. The force and the displacements are applied in the direction of the normal on the surface. The user must specify the normal underneath the *PRE-TENSION SECTION keyword. If the normal is specified away from the elements to which the surface belongs (volumetric case) or in the direction going from node 1 to node 2 in the element definition (for the beam element), a positive force or positive displacements correspond to tension in the underlying structure.

Notice that in the volumetric case the surface must be defined by element faces, it cannot be defined by nodes. Furthermore, the user should make sure that

- the surface does not contain edges or vertices of elements which do not have a face in common with the surface. Transgression of this rule will lead to unrealistic stress concentrations.
- the surface is not adjacent to quadratic elements adjacent to a slave or master contact surface. The latter elements are remeshed into linear elements. This remeshing is not taken into account in the definition of the

pre-tension multiple point constraint and will lead to unrealistic stress concentrations.

Internally, the nodes belonging to the element face surface are copied and a linear multiple point constraint is generated between the nodes expressing that the mean force is the force specified by the user (or similarly, the mean differential displacement is the one specified by the user). Therefore, if the user visualizes the results with CalculiX GraphiX, a gap will be noticed at the location of the pre-tension section.

For beam elements a linear multiple point constraint is created between the nodes belonging to the beam element. The beam element itself is deactivated,i.e. it will not show up in the frd-file.

First line:

- *PRE-TENSION SECTION
- Enter the NODE and the SURFACE or ELEMENT parameter and their values

Following line:

- First component in global coordinates of the normal on the surface
- Second component in global coordinates of the normal on the surface
- Third component in global coordinates of the normal on the surface

```
Example:

*PRE-TENSION SECTION,SURFACE=SURF1,NODE=234
1.,0.,0.
```

defines a pre-tension section consisting of the surface with the name SURF1 and reference node 234. The normal on the surface is defined as the positive global x-direction.

Example files: pret1, pret2, pret3.

7.81 *RADIATE

Keyword type: step

This option allows the specification of radiation heat transfer of a surface at absolute temperature θ (i.e. in Kelvin) and with emissivity ϵ to the environment at absolute temperature θ_0. The environmental temperature θ_0 is also called the sink temperature. If the user wishes so, it can be calculated by cavity radiation considerations from the temperatures of other visible surfaces. The radiation heat flux q satisfies:

$$q = \epsilon\sigma(\theta^4 - \theta_0^4), \tag{356}$$

where $\sigma = 5.67 \times 10^{-8} W/m^2K^4$ is the Stefan–Boltzmann constant. The emissivity takes values between 0 and 1. Blackbody radiation is characterized by $\epsilon = 1$. In CalculiX, the radiation is assumed to be diffuse (it does not depend on the angle under which it is emitted from the surface) and gray (it does not depend on the wavelength of the radiation). Selecting radiation type flux requires the inclusion of the *PHYSICAL CONSTANTS card, which specifies the value of the Stefan–Boltzmann constant and the value of absolute zero in the user's units. In order to specify which face the flux is entering or leaving the faces are numbered. The numbering depends on the element type.

For hexahedral elements the faces are numbered as follows (numbers are node numbers):

- Face 1: 1-2-3-4
- Face 2: 5-8-7-6
- Face 3: 1-5-6-2
- Face 4: 2-6-7-3
- Face 5: 3-7-8-4
- Face 6: 4-8-5-1

for tetrahedral elements:

- Face 1: 1-2-3
- Face 2: 1-4-2
- Face 3: 2-4-3
- Face 4: 3-4-1

and for wedge elements:

- Face 1: 1-2-3
- Face 2: 4-5-6
- Face 3: 1-2-5-4
- Face 4: 2-3-6-5
- Face 5: 3-1-4-6

for quadrilateral plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-4

- Face 4: 4-1
- Face N: in negative normal direction (only for plane stress)
- Face P: in positive normal direction (only for plane stress)

for triangular plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-1
- Face N: in negative normal direction (only for plane stress)
- Face P: in positive normal direction (only for plane stress)

for quadrilateral shell elements:

- Face NEG or 1: in negative normal direction
- Face POS or 2: in positive normal direction
- Face 3: 1-2
- Face 4: 2-3
- Face 5: 3-4
- Face 6: 4-1

for triangular shell elements:

- Face NEG or 1: in negative normal direction
- Face POS or 2: in positive normal direction
- Face 3: 1-2
- Face 4: 2-3
- Face 5: 3-1

The labels NEG and POS can only be used for uniform, non-cavity radiation and are introduced for compatibility with ABAQUS. Notice that the labels 1 and 2 correspond to the brick face labels of the 3D expansion of the shell (Figure 61).

for beam elements:

- Face 1: in negative 1-direction
- Face 2: in positive 1-direction
- Face 3: in positive 2-direction

- Face 5: in negative 2-direction

The beam face numbers correspond to the brick face labels of the 3D expansion of the beam (Figure 66).

Radiation flux characterized by a uniform emissivity is entered by the distributed flux type label Rx where x is the number of the face, followed by the sink temperature and the emissivity. If the emissivity is nonuniform the label takes the form RxNUy and a user subroutine radiate.f must be provided specifying the value of the emissivity and the sink temperature. The label can be up to 17 characters long. In particular, y can be used to distinguish different nonuniform emissivity patterns (maximum 13 characters).

If the user does not know the sink temperature but rather prefers it to be calculated from the radiation from other surfaces, the distributed flux type label RxCR should be used (CR stands for cavity radiation). In that case, the temperature immediately following the label is considered as environment temperature for viewfactors smaller than 1, what is lacking to reach the value of one is considered to radiate towards the environment. Sometimes, it is useful to specify that the radiation is closed. This is done by specifying a value of the environment temperature which is negative if expressed on the absolute scale (Kelvin). Then, the viewfactors are scaled to one exactly. For cavity radiation the sink temperature is calculated based on the interaction of the surface at stake with all other cavity radiation surfaces (i.e. with label RyCR, y taking a value between 1 and 6). Surfaces for which no cavity radiation label is specified are not used in the calculation of the viewfactor and radiation flux. Therefore, it is generally desirable to specify cavity radiation conditions on ALL element faces (or on none). If the emissivity is nonuniform, the label reads RxCRNUy and a subroutine radiate.f specifying the emissivity must be provided. The label can be up to 17 characters long. In particular, y can be used to distinguish different nonuniform emissivity patterns (maximum 11 characters).

Optional parameters are OP, AMPLITUDE, TIME DELAY, RADIATION AMPLITUDE, RADIATION TIME DELAY, ENVNODE and CAVITY. OP takes the value NEW or MOD. OP=MOD is default and implies that the radiation fluxes on different faces are kept over all steps starting from the last perturbation step. Specifying a radiation flux on a face for which such a flux was defined in a previous step replaces this value. OP=NEW implies that all previous radiation flux is removed. If multiple *RADIATE cards are present in a step this parameter takes effect for the first *RADIATE card only.

The AMPLITUDE parameter allows for the specification of an amplitude by which the sink temperature is scaled (mainly used for dynamic calculations). Thus, in that case the sink temperature values entered on the *RADIATE card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference value is replaced by the actual value at that time. In subsequent steps this value is kept constant unless it is explicitly redefined or the amplitude is defined using TIME=TOTAL TIME in which case the amplitude keeps its validity. The AMPLITUDE parameter has no effect on nonuniform fluxes and cavity

radiation.

The TIME DELAY parameter modifies the AMPLITUDE parameter. As such, TIME DELAY must be preceded by an AMPLITUDE name. TIME DELAY is a time shift by which the AMPLITUDE definition it refers to is moved in positive time direction. For instance, a TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The TIME DELAY parameter must only appear once on one and the same keyword card.

The RADIATION AMPLITUDE parameter allows for the specification of an amplitude by which the emissivity is scaled (mainly used for dynamic calculations). Thus, in that case the emissivity values entered on the *RADIATE card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference value is replaced by the actual value at that time. In subsequent steps this value is kept constant unless it is explicitly redefined or the amplitude is defined using TIME=TOTAL TIME in which case the amplitude keeps its validity. The RADIATION AMPLITUDE parameter has no effect on nonuniform fluxes.

The RADIATION TIME DELAY parameter modifies the RADIATION AMPLITUDE parameter. As such, RADIATION TIME DELAY must be preceded by an RADIATION AMPLITUDE name. RADIATION TIME DELAY is a time shift by which the RADIATION AMPLITUDE definition it refers to is moved in positive time direction. For instance, a RADIATION TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The RADIATION TIME DELAY parameter must only appear once on one and the same keyword card.

The ENVNODE option applies for uniform radiation conditions only and allows the user to specify a sink node instead of a sink temperature. In that case, the sink temperature is defined as the temperature of the sink node.

Finally, the CAVITY parameter can be used to separate closed cavities. For the calculation of the viewfactors for a specific face, only those faces are considered which:

- are subject to cavity radiation
- belong to the same cavity.

The name of the cavity can consist of maximum 3 characters (including numbers). Default cavity is ' ' (empty name). Since the calculation of the viewfactors is approximate, it can happen that, even if a cavity is mathematically closed, radiation comes in from outside. To prevent this, one can define the faces of the cavity as belonging to one and the same cavity, distinct from the cavities other faces belong to.

First line:

- *RADIATE
- Enter any needed parameters and their value

Following line for uniform, explicit radiation conditions:

- Element number or element set label.
- Radiation flux type label (Rx).
- Sink temperature, or, if ENVNODE is active, the sink node.
- Emissivity.

Repeat this line if needed.

Following line for nonuniform, explicit radiation conditions:

- Element number or element set label.
- Radiation flux type label (RxNUy).

Repeat this line if needed.

Following line for cavity radiation conditions with uniform emissivity and sink temperature:

- Element number or element set label.
- Radiation flux type label (RxCR).
- Sink temperature, or, if ENVNODE is active, the sink node.
- Emissivity.

Repeat this line if needed.

Following line for cavity radiation conditions with nonuniform emissivity and sink temperature:

- Element number or element set label.
- Radiation flux type label (RxCRNy).

Repeat this line if needed.

`Example:`

```
*RADIATE
20,R1,273.,.5
```

assigns a radiation flux to face 1 of element 20 with an emissivity of 0.5 and a sink temperature of 273.

Example files: oneel8ra, beamhtcr.

7.82 *RESTART

Keyword type: prestep (*RESTART,READ), step (*RESTART,WRITE)

Sometimes you wish to continue a previous run without having to redo the complete calculation. This is where the *RESTART keyword comes in. It can be used to store results for a later restart, or to continue a previous calculation.

There is one required parameter specifying whether you want to read previous results (READ) or store the results of the present calculation for future restarts (WRITE). This parameter must follow immediately after the *RESTART keyword card.

If you specify READ, you can indicate with the parameter STEP which step of the previous run is to be read. Default is one. The results will be read from the binary file "jobname.rin" which should have been generated in a previous run. A restart file can contain any number of steps and anything which is allowed within a step. For instance, one can define new loads based on sets generated in previous runs. If present, the *RESTART,READ line must be the first non-comment line in the input deck.

If you specify WRITE, you can specify the frequency (parameter FREQUENCY) at which results are stored. A frequency of two means that the results of every second step will be stored. Default is one. The results will be stored in binary format in file "jobname.rout". Any existing file with this name will be deleted prior to the first writing operation. For a subsequent restart job with name "jobname_new.inp" the "jobname.rout" file must be renamed into "jobname_new.rin". The *RESTART,WRITE combination must be used within a *STEP definition

First and only line:

- *RESTART
- Enter any needed parameters and their values

```
Example:

*RESTART,READ,STEP=2
```

will read the results of step two in the previous calculation.

```
Example:

*RESTART,WRITE,FREQUENCY=3
```

will write the results every third step.

Example files: beamread, beamwrite.

7.83 *RETAINED NODAL DOFS

Keyword type: step

This option is used to prescribe the nodal degrees of freedom which are kept in a *SUBSTRUCTURE GENERATE analysis. It cannot be used in any other sort of analysis.

There is one optional parameter: SORTED=NO. It is not possible to request a sorting of the degrees of freedom entered. The entries in the substructure stiffness matrix are in the order introduced by the user.

No transformation is allowed. Consequently, the global Carthesian system applies.

First line:

- *RETAINED NODAL DOFS
- Enter the parameter SORTED=NO (optional).

Following line:

- Node number or node set label
- First degree of freedom retained
- Last degree of freedom retained. This field may be left blank if only one degree of freedom is retained.

Repeat this line if needed.

Example:

```
*RETAINED NODAL DOFS
73,1,3
```

retains the degrees of freedom one through three (global) of node 73.

Example files: substructure.

7.84 *RIGID BODY

Keyword type: model definition

With this card a rigid body can be defined consisting of nodes or elements. Optional parameters are REF NODE and ROT NODE.

One of the parameters NSET or ELSET is required. Use NSET to define a rigid body consisting of the nodes belonging to a node set and ELSET for a rigid body consisting of the elements belonging to an element set. In the latter case, the rigid body really consists of the nodes belonging to the elements. The parameters NSET and ELSET are mutually exclusive. The rigid body definition ensures that the distance between any pair of nodes belonging to the body does

not change during deformation. This means that the degrees of freedom are reduced to six: three translational and three rotational degrees of freedom. Thus, the motion is reduced to a translation of a reference node and a rotation about that node.

The reference node can be specified by the parameter REF NODE and should have been assigned coordinates using the *NODE card. The reference node can belong to the rigid body, but does not necessarily have to. Notice, however, that if the reference node belongs to the rigid body any forces requested by specifying RF on a *NODE PRINT card will not be correct.

For the rotational degrees of freedom a dummy rotational node is used whose translational degrees of freedom are interpreted as the rotations about the reference node. Thus, the first degree of freedom is used as the rotation about the x-axis of the rigid body, the second as the the rotation about the y-axis and the third as the rotation about the z-axis. The rotational node can be defined explicitly using the parameter ROT NODE. In that case, this node must be been assigned coordinates (their value is irrelevant) and should not belong to any element of the structure.

In the absence of any of the parameters REF NODE or ROT NODE, extra nodes are generated internally assuming their tasks. The position of the default REF NODE is the origin. However, defining the nodes explicitly can be useful if a rotation about a specific point is to be defined (using *BOUNDARY or *CLOAD), or if rigid body values (displacements or forces) are to be printed using *NODE PRINT. Notice that a force defined in a rotational node has the meaning of a moment.

Internally, a rigid body is enforced by using nonlinear multiple point constraints (MPC).

If the participating nodes in a rigid body definition lie on a straight line, the rigid body rotation about the line is not defined and an error will occur. To remove the rotational degree of freedom, specify that the rotation about the axis is zero. If $\mathbf{a}$ is a unit normal on the axis and $\mathbf{u}_R$ is the displacement of the ROT NODE, this results in a linear MPC of the form $\mathbf{a}.\mathbf{u}_R = 0$ to be specified by the user by means of a *EQUATION card.

First and only line:

- *RIGID BODY
- Enter any needed parameters and their values

```
Example:

*RIGID BODY,NSET=rigid1,REF NODE=100,ROT NODE=101
```

defines a rigid body consisting of the nodes belonging to node set rigid1 with reference node 100 and rotational node 101.

Using

```
*CLOAD
101,3,0.1
```

in the same input deck (see *CLOAD) defines a moment about the z-axis of 0.1 acting on the rigid body.

Example files: beamrb.

7.85 *SELECT CYCLIC SYMMETRY MODES

Keyword type: step

This option is used to trigger an eigenmode analysis for cyclic symmetric structures. It must be preceded by a *FREQUENCY card. There are two optional parameters NMIN, NMAX. NMIN is the lowest cyclic symmetry mode number (also called nodal diameter)to be considered (default 0), NMAX is the highest cyclic symmetry mode number (default N/2 for N even and (N+1)/2 for N odd, where N is the number of sectors on the *CYCLIC SYMMETRY MODEL card.

For models containing the axis of cyclic symmetry (e.g. a full disk), the nodes on the symmetry axis are treated differently depending on whether the cyclic symmetry mode number is 0, 1 or exceeds 1. Therefore, for such structures calculations for cyclic symmetry mode numbers 0 or 1 must be performed in separate steps with NMIN=0,NMAX=0 and NMIN=1,NMAX=1, respectively.

First and only line:

- *SELECT CYCLIC SYMMETRY MODES
- Enter the parameters NMIN and NMAX and their values, if appropriate.

Example:

```
*SELECT CYCLIC SYMMETRY MODES, NMIN=2, NMAX=4
```

triggers a cyclic symmetry calculation for mode numbers 2 up to and including 4.

Example files: segment, fullseg.

7.86 *SHELL SECTION

Keyword type: model definition

This option is used to assign material properties to shell element sets. The parameter ELSET is required, one of the mutually exclusive parameters MATERIAL and COMPOSITE is required too, whereas the parameters ORIENTATION, NODAL THICKNESS, OFFSET are optional. The parameter ELSET

defines the shell element set to which the material specified by the parameter MATERIAL applies. The parameter ORIENTATION allows to assign local axes to the element set. If activated, the material properties are applied to the local axis. This is only relevant for non isotropic material behavior. The parameter NODAL THICKNESS indicates that the thickness for ALL nodes in the element set are defined with an extra *NODAL THICKNESS card and that any thicknesses defined on the *SHELL SECTION card are irrelevant. The OFFSET parameter indicates where the mid-surface of the shell should be in relation to the reference surface defined by the surface representation given by the user. The unit of the offset is the thickness of the shell. Thus, OFFSET=0 means that the reference surface is the mid-surface of the shell, OFFSET=0.5 means that the reference surface is the top surface of the shell. The offset can take any real value. Finally, the COMPOSITE parameter is used to define a composite material. It can only be used for S8R elements. A composite material consists of an integer number of layers made up of different materials with possibly different orientations. For a composite material the material is specified on the lines beneath the *SHELL SECTION card for each layer separately. The orientation for each layer can be specified in the same way. If none is specified, the orientation defined by the ORIENTATION parameter will be taken, if any.

First line:

- *SHELL SECTION
- Enter any needed parameters.

Second line if the parameter COMPOSITE is not used (only read if the first line does not contain NODAL THICKNESS):

- thickness

Second line if the parameter COMPOSITE is used (NODAL THICKNESS is not allowed):

- thickness (required)
- not used
- name of the material to be used for this layer (required)
- name of the orientation to be used for this layer (optional)

Repeat this line as often as needed to define all layers.

```
Example:

*SHELL SECTION,MATERIAL=EL,ELSET=Eall,ORIENTATION=OR1,OFFSET=-0.5
3.
```

assigns material EL with orientation OR1 to all elements in (element) set Eall. The reference surface is the bottom surface of the shell and the shell thickness is 3 length units.

Example files: shell1, shell2, shellbeam.

7.87 *SOLID SECTION

Keyword type: model definition

This option is used to assign material properties to 3D, plane stress, plane strain and axisymmetric element sets. The parameters ELSET and MATERIAL are required, the parameter ORIENTATION is optional. The parameter ELSET defines the element set to which the material specified by the parameter MATERIAL applies. The parameter ORIENTATION allows to assign local axes to the element set. If activated, the material properties are applied to the local axis. This is only relevant for non isotropic material behavior. For plane stress and plane strain elements the thickness can be specified on the second line. Default is 1.

First line:

- *SOLID SECTION
- Enter any needed parameters.

Second line (only relevant for plane stress, plane strain and axisymmetric elements; can be omitted for 3D elements):

- thickness (plane stress and plane strain elements)

```
Example:

*SOLID SECTION,MATERIAL=EL,ELSET=Eall,ORIENTATION=OR1
```

assigns material EL with orientation OR1 to all elements in (element) set Eall.

Example files: beampo2, planestress.

7.88 *SPECIFIC GAS CONSTANT

Keyword type: model definition, material

With this option the specific gas constant of a material can be defined. The specific gas constant is required for a calculation in which a gas dynamic network is included. The specific gas constant R is defined as

$$R = \mathcal{R}/M \tag{357}$$

where $\mathcal{R} = 8314$ J/(kmol K) is the universal gas constant and M is the molecular weight of the material. The specific gas constant is temperature independent.

First line:

- *SPECIFIC GAS CONSTANT

Following line:

- Specific gas constant.

Example:

```
*SPECIFIC GAS CONSTANT
287.
```

defines a specific gas constant with a value of 287. This value is appropriate for air if Joule is chosen for the unit of energy, kg as unit of mass and K as unit of temperature, i.e. $R = 287$ J/(kg K).

Example files: linearnet, branch1, branch2.

7.89 *SPECIFIC HEAT

Keyword type: model definition, material

With this option the specific heat of a solid material can be defined. The specific heat is required for a transient heat transfer analysis (*HEAT TRANSFER or *COUPLED TEMPERATURE-DISPLACEMENT). The specific heat can be temperature dependent.

This option should not be used to define the specific heat of a fluid (gas or liquid) in an aerodynamic or fluid dynamic network. For the latter purpose the keyword *FLUID CONSTANTS is available.

First line:

- *SPECIFIC HEAT

Following line:

- Specific heat.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Example:

```
*SPECIFIC HEAT
446.E6
```

defines a specific heat with value $446. \times 10^6$ for all temperatures.

Example files: beamth, beamhtcr.

7.90 *SPRING

Keyword type: model definition

With this option the force-displacement relationship can be defined for spring elements. There is one required parameter ELSET and one optional parameter NONLINEAR. With the parameter ELSET the element set is referred to for which the spring behavior is defined. This element set should contain spring elements of type SPRINGA only. With the parameter NONLINEAR the user can specify that the behavior of the spring is nonlinear, default is a linear behavior.

Please note that for a nonlinear behavior the (force,elongation) pairs have to be entered in ascending order of the elongation. The elongation is defined as the final length minus the initial length. The elongation can be negative, however, it should not be smaller than the initial length of the spring. Extrapolation in the force versus elongation graph is done in a constant way, i.e. the force is kept constant. This leads to a zero tangent and may lead to a singular stiffness matrix. Therefore, the elongation range should be defined large enough to avoid this type of problems.

First line:

- *SPRING
- Enter the parameter ELSET and its value

Second line: enter a blank line

Following line if the parameter NONLINEAR is not used:

- Spring constant.
- not used.
- Temperature.

Repeat this line if needed to define complete temperature dependence.

Following sets of lines define the force-displacement curve if the parameter NONLINEAR is active: First line in the first set:

- Spring force.
- Elongation.
- Temperature.

Use as many lines in the first set as needed to define the complete force-displacement curve for this temperature.

Use as many sets as needed to define complete temperature dependence.

Example:

```
*SPRING,ELSET=Eall
10.
```

defines a linear spring constant with value 10. for all elements in element set Eall and all temperatures.

Example:

```
*SPRING,ELSET=Eall,NONLINEAR
0.,0.,293.
10.,1.,293.
100.,2.,293.
0.,0.,393.
5.,1.,393.
25.,2.,393.
```

defines a nonlinear spring characterized by a force-displacement curve through (0,0),(10,1),(100,2) for a temperature of 293. and through (0,0),(5,1),(25,2) for a temperature of 393. The first scalar in the couples is the force, the second is the elongation of the spring. This spring behavior applies to all elements in element set Eall. Notice that for displacements outside the defined range the force is kept constant. For instance, in the example above the force for an elongation of 3 at a temperature of 293 will be 100.

Example files: spring1, spring2, spring3, spring4, spring5.

7.91 *STATIC

Keyword type: step

This procedure is used to perform a static analysis. The load consists of the sum of the load of the last *STATIC step and the load specified in the present step with replacement of redefined loads. This card is also correct for steady state incompressible flow calculations without heat transfer.

There are five optional parameters: SOLVER, DIRECT, EXPLICIT, TIME RESET and TOTAL TIME AT START. SOLVER determines the package used to solve the ensuing system of equations. The following solvers can be selected:

- the SGI solver
- PARDISO
- SPOOLES [3, 4].
- TAUCS
- the iterative solver by Rank and Ruecker [60], which is based on the algorithms by Schwarz [64].

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, the default is the iterative solver, which comes with the CalculiX package.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU decomposition, however, I was not able to run either of them so far. Next comes the iterative solver. If SOLVER=ITERATIVE SCALING is selected, the pre-conditioning is limited to a scaling of the diagonal terms, SOLVER=ITERATIVE CHOLESKY triggers Incomplete Cholesky pre-conditioning. Cholesky pre-conditioning leads to a better convergence and maybe to shorter execution times, however, it requires additional storage roughly corresponding to the non-zeros in the matrix. If you are short of memory, diagonal scaling might be your last resort. The iterative methods perform well for truly three-dimensional structures. For instance, calculations for a hemisphere were about nine times faster with the ITERATIVE SCALING solver, and three times faster with the ITERATIVE CHOLESKY solver than with SPOOLES. For two-dimensional structures such as plates or shells, the performance might break down drastically and convergence often requires the use of Cholesky preconditioning. SPOOLES (and any of the other direct solvers) performs well in most situations with emphasis on slender structures but requires much more storage than the iterative solver. PARDISO is the Intel proprietary solver.

The parameter DIRECT is relevant for nonlinear calculations only, and indicates that automatic incrementation should be switched off.

The parameter EXPLICIT is only important for fluid computations. If present, the fluid computation is explicit, else it is semi-implicit. Static structural computations are always implicit.

The parameter TIME RESET can be used to force the total time at the end of the present step to coincide with the total time at the end of the previous step. If there is no previous step the targeted total time is zero. If this parameter is absent the total time at the end of the present step is the total time at the end of the previous step plus the time period of the present step (2nd parameter underneath the *STATIC keyword). Consequently, if the time at the end of the previous step is 10. and the present time period is 1., the total time at the end of the present step is 11. If the TIME RESET parameter is used, the total time at the beginning of the present step is 9. and at the end of the present step it will be 10. This is sometimes useful if thermomechanical calculations are split into transient heat transfer steps followed by quasi-static static steps (this can be faster than using the *COUPLED TEMPERATURE-DISPLACEMENT option, which forces the same amount of iterations for the thermal as for the mechanical calculations and than using the *UNCOUPLED TEMPERATURE-DISPLACEMENT option, which forces the same amount of increments for the

thermal as for the mechanical calculations). In CalculiX the static step needs a finite time period, however, the user frequently does not want the quasi-static step to change the time count.

Finally, the parameter TOTAL TIME AT START can be used to set the total time at the start of the step to a specific value.

In a static step, loads are by default applied in a linear way. Other loading patterns can be defined by an *AMPLITUDE card.

If nonlinearities are present in the model (geometric nonlinearity or material nonlinearity), the solution is obtained through iteration. Since the step may be too large to obtain convergence, a subdivision of the step in increments is usually necessary. The user can define the length of the initial increment. This size is kept constant if the parameter DIRECT is selected, else it is varied by CalculiX according to the convergence properties of the solution. In a purely linear calculation the step size is always 1., no iterations are performed and, consequently, no second line underneath *STATIC is needed.

Notice that any creep behavior (e.g. by using the keyword *CREEP) is switched off in a *STATIC step. To include creep use the *VISCO keyword. The syntax for both keywords is the same.

First line:

- *STATIC
- Enter any needed parameters and their values.

Second line (only relevant for nonlinear analyses; for linear analyses, the step length is always 1)

- Initial time increment. This value will be modified due to automatic incrementation, unless the parameter DIRECT was specified (default 1.).
- Time period of the step (default 1.).
- Minimum time increment allowed. Only active if DIRECT is not specified. Default is the initial time increment or 1.e-5 times the time period of the step, whichever is smaller.
- Maximum time increment allowed. Only active if DIRECT is not specified. Default is 1.e+30.
- Initial time increment for CFD applications (default 1.e-2)

Example:

```
*STATIC,DIRECT
.1,1.
```

defines a static step and selects the SPOOLES solver as linear equation solver in the step (default). If the step is a linear one, the other parameters are of no importance. If the step is nonlinear, the second line indicates that the initial time increment is .1 and the total step time is 1. Furthermore, the parameter DIRECT leads to a fixed time increment. Thus, if successful, the calculation consists of 10 increments of length 0.1.

Example files: beampic, beampis.

7.92 *STEADY STATE DYNAMICS

Keyword type: step

This procedure is used to calculate the steady state response of a structure subject to periodic loading. Although the deformation up to the onset of the dynamic calculation can be nonlinear, this procedure is basically linear and assumes that the response can be written as a linear combination of the lowest modes of the structure. To this end, these modes must have been calculated in a previous *FREQUENCY,STORAGE=YES step (not necessarily in the same calculation). In the *STEADY STATE DYNAMICS step the eigenfrequencies, modes, stiffness and mass matrix are recovered from the file jobname.eig.

For harmonic loading the steady state response is calculated for the frequency range specified by the user. The number of data points within this range n can also be defined by the user, default is 20, minimum is 2 (if the user specifies n to be less than 2, the default is taken). If no eigenvalues occur within the specified range, this is the total number of data points taken, i.e. including the lower frequency bound and the upper frequency bound. If one or more eigenvalues fall within the specified range, $n-2$ points are taken in between the lower frequency bound and the lowest eigenfrequency in the range, $n-2$ between any subsequent eigenfrequencies in the range and $n-2$ points in between the highest eigenfrequency in the range and upper frequency bound. Consequently, if m eigenfrequencies belong to the specified range, $(m+1)(n-2)+m+2 = nm-m+n$ data points are taken. They are equally spaced in between the fixed points (lower frequency bound, upper frequency bound and eigenfrequencies) if the user specifies a bias equal to 1. If a different bias is specified, the data points are concentrated about the fixed points. Default for the bias is 3., minimum value allowed is 1. (if the user specifies a value less than 1., the default is taken). The number of eigenmodes used is taken from the previous *FREQUENCY step. Since a steady state dynamics step is a perturbation step, all previous loading is removed. The loading defined within the step is multiplied by the amplitude history for each load as specified by the AMPLITUDE parameter on the loading card, if any. In this context the AMPLITUDE cards are interpreted as load factor versus frequency. Loading histories extending beyond the amplitude frequency scale are extrapolated in a constant way. The absence of the AMPLITUDE parameter on a loading card leads to a frequency independent load.

For nonharmonic loading the loading across one period is not harmonic and has to be specified in the time domain. To this end the user can specify the starting time and the final time of one period and describe the loading within this period with *AMPLITUDE cards. Default is the interval $[0., 1.]$ and step loading. Notice that for nonharmonic loading the *AMPLITUDE cards describe amplitude versus TIME. Furthermore, the user can specify the number of Fourier terms the nonharmonic loading is expanded in (default:20). The remaining input is the same as for harmonic loading, i.e. the user specifies a frequency range, the number of data points within this range and the bias.

There are two optional parameters: HARMONIC and SOLVER. HARMONIC=YES (default) indicates that the periodic loading is harmonic, HARMONIC=NO specifies nonharmonic periodic loading. The parameter SOLVER determines the package used to solve for the steady state solution in the presence of nonzero displacement boundary conditions. The following solvers can be selected:

- the SGI solver
- PARDISO
- SPOOLES [3, 4].
- TAUCS

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, an error is issued.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU decomposition, however, I was not able to run either of them so far. PARDISO is the Intel proprietary solver.

First line:

- *STEADY STATE DYNAMICS
- enter any of the parameters you need.

Second line for HARMONIC=YES (default):

- Lower bound of the frequency range (cycles/time)
- Upper bound of the frequency range (cycles/time)
- Number of data points n (default: 20)

- Bias (default: 3.)

Second line for HARMONIC=NO:

- Lower bound of the frequency range (cycles/time)
- Upper bound of the frequency range (cycles/time)
- Number of data points n (default: 20)
- Bias (default: 3.)
- Number of Fourier terms n (default: 20)
- Lower bound of the time range (default: 0.)
- Upper bound of the time range (default: 1.)

Example:

```
*STEADY STATE DYNAMICS
12000.,14000.,5,4.
```

defines a steady state dynamics procedure in the frequency interval [12000., 14000.] with 5 data points and a bias of 4.

Example:

```
*STEADY STATE DYNAMICS,HARMONIC=NO
2.,4.,3,1.,11,0.,.5
```

defines a steady state dynamics procedure in the time domain. A complete period is defined in the time interval [0.,0.5], and 11 Fourier terms will be taken. Calculations will be performed for three equidistant points in the frequency interval [2.,4.], i.e. for 2 cycles/time, 3 cycles/time and 4 cycles/time, provided there are no eigenfrequencies in this interval.

Example files: beamdy8, beamdy9, beamdy10, beamdy11, beamdy12, beamdy13.

7.93 *STEP

Keyword type: step

This card describes the start of a new STEP. PERTURBATION, NLGEOM, INC, INCF, TURBULENCE MODEL and SHOCK SMOOTHING are the optional parameters.

The parameter PERTURBATION is allowed for *FREQUENCY and *BUCKLE steps only. If it is specified, the last *STATIC step is taken as reference state and used to calculate the stiffness matrix. This means the inclusion of previous deformations (large deformation stiffness) and the inclusion of previous loads as preloads (stress stiffness), taking the temperatures into account to determine

the material properties. The loads active (mechanical and thermal) are those specified in the perturbation step. The displacements and stresses are those corresponding to the eigenmodes. At the end of the step the perturbation load is reset to zero.

The loading active in a non-perturbative step is the accumulation of the loading in all previous steps since but not including the last perturbation step (or, if none has occurred, since the start of the calculation), unless OP=NEW has been specified since.

If NLGEOM is specified, the calculation takes geometrically nonlinear effects into account. To this end a nonlinear strain tensor is used (Lagrangian strain for hyperelastic materials, Eulerian strain for deformation plasticity and the deviatoric elastic left Cauchy-Green tensor for incremental plasticity), the step is divided into increments and a Newton iteration is performed within each increment. Although the internally used stresses are the Piola stresses of the second kind, they are transformed into Cauchy (true) stresses before being printed. In the present version of the program geometrically nonlinear calculations only apply to static calculations, and consequently the *STATIC or *DYNAMIC keyword card should be used within the step. The latter card also allows for the specification of the step size and increment size. The maximum number of increments in the step (for automatic incrementation) can be specified by using the parameter INC (default is 100) for thermomechanical calculations and INCF (default is 10000) for 3D fluid calculations. In coupled fluid-structure calculations INC applies to the thermomechanical part of the computations and INCF to the 3D fluid part. Once the NLGEOM parameter has been selected, it remains active in all subsequent static calculations. Some analyses involving nonlinear materials (*HYPERELASTIC, *HYPERFOAM, *DEFORMATION PLASTICITY, *PLASTIC, *CREEP) automatically trigger the NLGEOM option. Thus, for these types of analysis nonlinear geometric effects are always taken into account. This also applies to analyses with 1d or 2d elements in the presence of knots and calculations with *GAP, *MPC or *RIGID BODY definitions.

For 3D fluid calculations the parameter TURBULENCE MODEL defines the turbulence model to be used. The user can choose among NONE (laminar calculations; this is default), K-EPSILON, K-OMEGA and SST [48]. In addition, if the flow is compressible, a shock smoothing coefficient can be chosen using the parameter SHOCK SMOOTHING. Its value should be in the range between 0.0 and 2.0. The larger this coefficient, the more the results are smoothed and the more likely the predictive quality of your calculation will be poor. Therefore, one should start a calculation with a zero shock smoothing coefficient (default). If this calculation converges and the results look fine, no further smoothing should be introduced. If the calculation does not converge are the solution looks totally wrong, the shock smooting coefficient should be increased until convergence with good quality results takes place. This coefficient does not have any impact on incompressible flow.

First and only line:

- *STEP
- Enter any needed parameters and their values

Example:

```
*STEP,INC=1000,INCF=20000,TURBULENCE MODEL=SST
```

starts a step and increases the maximum number of thermomechanical increments to complete the step to 1000. The maximum number of 3D fluid increments is set to 20000 and for the turbulence model the SST model was chosen.

Example files: beamnlp.

7.94 *SUBMODEL

Keyword type: model definition

This keyword is used to define submodel boundaries. A submodel is a part of a bigger model for which an analysis has already been performed. A submodel is used if the user would like to analyze some part in more detail by using a more dense mesh or a more complicated material model, just to name a few reasons. At those locations where the submodel has been cut from the global model, the boundary conditions are derived from the global model results. These are the boundaries defined by the *SUBMODEL card. In addition, in a purely mechanical calculation it allows to map the temperatures to all nodes in the submodel (not just the boundary nodes).

There are four kinds of boundary conditions one may apply: the user may map the displacements from the global model (or temperatures in a purely thermal or a thermo-mechanical calculation) to the boundaries of the submodel, the user may want to map the stresses to the boundaries of the submodel, the user may want to map the forces to the boundaries of the submodel or the user may select to map the temperatures in a purely mechanical calculation to all nodes belonging to the submodel. Mapping the stresses or forces may require fixing a couple of additional nodes to prevent rigid body modes.

In order to perform the mapping (which is basically an interpolation) the global model is remeshed with tetrahedra. The resulting mesh is stored in file TetMasterSubmodel.frd and can be viewed with CalculiX GraphiX.

There are three parameters of which two are required. The parameters TYPE and INPUT are required. TYPE can take the value SURFACE or NODE, depending on whether the user wants to define stress boundary conditions or displacement/temperature/force boundary conditions, respectively. The parameter INPUT specifies the file, in which the results of the global model are stored. This must be a .frd file.

A submodel of the SURFACE type is defined by element face surfaces. These must be defined using the *SURFACE,TYPE=ELEMENT card. Submodels of the NODE type are defined by sets of nodes. Several submodel cards may

be used in one and the same input deck, and they can be of different types. The global result file, however, must be the same for all *SUBMODEL cards. Furthermore, a node (for the NODE type submodel) or an element face (for the SURFACE type submodel) may only belong to at most one *SUBMODEL.

The optional parameter GLOBAL ELSET defines an elset in the global model which will be used for the interpolation of the displacements or stresses onto the submodel boundary defined underneath the *SUBMODEL card. Default is the complete global model. Global elsets of different *SUBMODEL cards may have elements in common.

Notice that the *SUBMODEL card only states that the model at stake is a submodel and that it defines part of the boundary to be of the nodal or of the surface type. Whether actually displacements or stresses will be applied by interpolation from the global model depends on whether a *BOUNDARY, SUBMODEL, *DSLOAD, *CLOAD, SUBMODEL or *TEMPERATURE, SUBMOBEL card is used, respectively.

Mapping displacements or temperatures to the boundary of a submodel is usually very accurate. For stresses, the results may be unsatisfactory, since the stress values stored in the global model (and which are the basis for the interpolation) are extrapolations of integration point values. This frequently leads to a situation in which equilibrium for the submodel is not satisfied. To circumvent this, the user may perform a submodel analysis with displacement boundary conditions, store the forces at the boundaries in the frd-file and use this file as global model for a subsequent submodel analysis with force boundary conditions. In this way a correct force-driven analysis can be performed, for instance for crack propagation analyses in the submodel (displacement-driven analyses prevent the crack from growing).

First line:

- *SUBMODEL
- Enter the parameters TYPE and INPUT and their value, and, if necessary, the GLOBAL ELSET parameter.

Following line for TYPE=NODE:

- Node or node set to be assigned to this surface (maximum 16 entries per line).

Repeat this line if needed.

Following line for TYPE=SURFACE:

- Element face surface (maximum 1 entry per line).

Repeat this line if needed.

Example:

```
*SUBMODEL,TYPE=NODE,INPUT=global.frd
```

```
part,
1,
8
```

states the the present model is a submodel. The nodes with number 1, and 8 and the nodes belong to a Dirichlet part of the boundary, i.e. a part on which the displacements may be obtained from the global model. The results of the global model are stored in file global.frd. Whether they are really used, depends on whether a *BOUNDARY,SUBMODEL card is defined for these nodes.

Example files: .

7.95 *SUBSTRUCTURE GENERATE

Keyword type: step

This procedure is used to generate a substructure and store the stiffness matrix using the *SUBSTRUCTURE MATRIX OUTPUT keyword card. No loading should be applied.

There is one optional parameter: SOLVER. It determines the package used to solve the ensuing system of equations. The following solvers can be selected:

- PARDISO
- SPOOLES [3, 4].

Default is the first solver which has been installed of the following list: PARDISO, SPOOLES. If none is installed, a substructure generation is not possible.

First line:

- *SUBSTRUCTURE GENERATE
- Enter SOLVER, if needed, and its value.

```
Example:

*SUBSTRUCTURE GENERATE,SOLVER=PARDISO
```

defines a substructure generation step and selects the PARDISO solver as linear equation solver in the step. For this to work, the PARDISO solver must have been linked with CalculiX.

Example files: substructure.

7.96 *SUBSTRUCTURE MATRIX OUTPUT

Keyword type: step

This option is used to define the name of the file in which the stiffness matrix of the substructure is to be stored which was generated within a *SUBSTRUCTURE GENERATE step. This is the only procedure in which this keyword card makes sense.

There are two optional parameters STIFFNESS and OUTPUT FILE, and one required parameter FILE NAME.

The optional parameters can only take a fixed value: STIFFNESS=YES and OUTPUT FILE= USER DEFINED. No other value is allowed.

The required parameter FILE NAME is used to define the name of the file in which the stiffness is to be stored. The extension .mtx is default and cannot be changed. It is automatically appended to the name given by the user.

First line:

- *SUBSTRUCTURE MATRIX OUTPUT
- Enter the parameter FILE NAME and its name, and optionally, the parameters STIFFNESS and OUTPUT FILE with their fixed values.

```
Example:

*SUBSTRUCTURE MATRIX OUTPUT,FILE NAME=substruc
```

defines file substruc.mtx for the storage of the substructure stiffness matrix.

Example files: substructure.

7.97 *SURFACE

Keyword type: model definition

This option is used to define surfaces made up of nodes or surfaces made up of element faces. A mixture of nodes and element faces belonging to one and the same surface is not possible. There are two parameters: NAME and TYPE. The parameter NAME containing the name of the surface is required. The TYPE parameter takes the value NODE for nodal surfaces and ELEMENT for element face surfaces. Default is TYPE=ELEMENT.

At present, surfaces are used to establish cyclic symmetry conditions and to define contact (including tied contact). The master and slave surfaces in cyclic symmetry conditions must be nodal surfaces. For contact, the slave surface can be a nodal or element face surface, while the master surface has to be a element face surface.

Element faces are identified by the surface label Sx where x is the number of the face. The numbering depends on the element type.

For hexahedral elements the faces are numbered as follows (numbers are node numbers):

- Face 1: 1-2-3-4
- Face 2: 5-8-7-6
- Face 3: 1-5-6-2
- Face 4: 2-6-7-3
- Face 5: 3-7-8-4
- Face 6: 4-8-5-1

for tetrahedral elements:

- Face 1: 1-2-3
- Face 2: 1-4-2
- Face 3: 2-4-3
- Face 4: 3-4-1

and for wedge elements:

- Face 1: 1-2-3
- Face 2: 4-5-6
- Face 3: 1-2-5-4
- Face 4: 2-3-6-5
- Face 5: 3-1-4-6

for quadrilateral plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-4
- Face 4: 4-1
- Face N: in negative normal direction (only for plane stress)
- Face P: in positive normal direction (only for plane stress)

for triangular plane stress, plane strain and axisymmetric elements:

- Face 1: 1-2
- Face 2: 2-3
- Face 3: 3-1

- Face N: in negative normal direction (only for plane stress)
- Face P: in positive normal direction (only for plane stress)

for quadrilateral shell elements:

- Face NEG or 1: in negative normal direction
- Face POS or 2: in positive normal direction
- Face 3: 1-2
- Face 4: 2-3
- Face 5: 3-4
- Face 6: 4-1

for triangular shell elements:

- Face NEG or 1: in negative normal direction
- Face POS or 2: in positive normal direction
- Face 3: 1-2
- Face 4: 2-3
- Face 5: 3-1

Notice that the labels 1 and 2 correspond to the brick face labels of the 3D expansion of the shell (Figure 61).

for beam elements:

- Face 1: in negative 1-direction
- Face 2: in positive 1-direction
- Face 3: in positive 2-direction
- Face 5: in negative 2-direction

The beam face numbers correspond to the brick face labels of the 3D expansion of the beam (Figure 66).

First line:

- *SURFACE
- Enter the parameter NAME and its value, and, if necessary, the TYPE parameter.

Following line for nodal surfaces:

- Node or node set to be assigned to this surface (maximum 1 entry per line).

Repeat this line if needed.

Following line for element face surfaces:

- Element or element set (maximum 1 entry per line).
- Surface label (maximum 1 entry per line).

Repeat this line if needed.

```
Example:

*SURFACE,NAME=left,TYPE=NODE
part,
1,
8
```

assigns the nodes with number 1, and 8 and the nodes belonging to node set part to a surface with name left.

```
Example:

*SURFACE,NAME=new
38,S6
```

assigns the face 6 of element 38 to a surface with name new.

Example files: segment, fullseg.

7.98 *SURFACE BEHAVIOR

Keyword type: model definition, surface interaction

With this option the surface behavior of a surface interaction can be defined. The surface behavior is required for a contact analysis. There is one required parameter PRESSURE-OVERCLOSURE. It can take the value EXPONENTIAL, LINEAR, TABULAR or TIED.

The exponential pressure-overclosure behavior takes the form in Figure 113. The parameters c_0 and p_0 define the kind of contact. p_0 is the contact pressure at zero distance, c_0 is the distance from the master surface at which the pressure is decreased to 1 % of p_0. The behavior in between is exponential. A large value of c_0 leads to soft contact, a small value to hard contact.

The linear pressure-overclosure behavior (Figure 114) simulates a linear relationship between the pressure and the overclosure. At zero overclosure the pressure is zero as well. For node-to-face penalty contact the user has to specify the slope of the pressure-overclosure curve and the tension value for large clearances σ_∞ (should be small, typically 0.25 % of the maximum stress expected). The value of c_0, which relates to the maximum clearance for which a

spring contact element is generated can be specified too (default value 10^{-3}). For face-to-face contact only the slope of the pressure-overclosure relationship is needed.

The tabular pressure-overclosure relationsship is a piecewise linear curve. The user enters (pressure,overclosure) pairs. Outside the interval specified by the user the pressure stays constant. The value of c_0, which relates to the maximum clearance for which a spring contact element is generated takes the value 10^{-3} and cannot be changed by the user.

The tied pressure-overclosure behavior simulates a truly linear relationship between the pressure and the overclosure for positive and negative pressures. At zero overclosure the pressure is zero. It can only be used for face-to-face contact and similates tied contact between the slave and master face. The only parameter is the slope of the pressure-overclosure relationship.

First line:

- *SURFACE BEHAVIOR
- Enter the parameter PRESSURE-OVERCLOSURE and its value.

Following line if PRESSURE-OVERCLOSURE=EXPONENTIAL:

- c_0.
- p_0.

Following line if PRESSURE-OVERCLOSURE=LINEAR:

- slope K of the pressure-overclosure curve (> 0).
- σ_∞ (> 0, irrelevant vor face-to-face contact).
- c_0 (> 0, irrelevant for face-to-face contact, optional for node-to-face contact)

Following line if PRESSURE-OVERCLOSURE=TABULAR:

- pressure.
- overclosure.

Repeat this line as often as needed.

Following line if PRESSURE-OVERCLOSURE=TIED:

- slope K of the pressure-overclosure curve (> 0).

`Example:`

```
*SURFACE BEHAVIOR,PRESSURE-OVERCLOSURE=EXPONENTIAL
1.e-4,.1
```

defines a distance of 10^{-4} length units at which the contact pressure is .001 pressure units, whereas the contact pressure at loose contact is 0.1 pressure units.

Example files: contact1, contact2.

7.99 *SURFACE INTERACTION

Keyword type: model definition

This option is used to start a surface interaction definition. A surface interaction data block is defined by the options between a *SURFACE INTERACTION line and either another *SURFACE INTERACTION line or a keyword line that does not define surface interaction properties. All surface interaction options within a data block will be assumed to define the same surface interaction. If a property is defined more than once for a surface interaction, the last definition is used. There is one required parameter, NAME, defining the name of the surface interaction with which it can be referenced in surface interactions (e.g. *CONTACT PAIR). The name can contain up to 80 characters.

If used for penalty contact the surface interaction definition must contain a *SURFACE BEHAVIOR card.

Surface interaction data requests outside the defined ranges are extrapolated in a constant way. Be aware that this occasionally occurs due to rounding errors.

First line:

- *SURFACE INTERACTION
- Enter the NAME parameter and its value.

Example:

```
*SURFACE INTERACTION,NAME=SI1
```

starts a material block with name SI1.

Example files: contact1, contact2.

7.100 *TEMPERATURE

Keyword type: step

This option is used to define temperatures and, for shell and beam elements, temperature gradients within a purely mechanical *STEP definition. *TEMPERATURE should not be used within a pure thermal or combined thermomechanical analysis. In these types of analysis the *BOUNDARY card for degree of freedom 11 should be used instead.

Optional parameter are OP, AMPLITUDE, TIME DELAY, USER, SUBMODEL and STEP. OP can take the value NEW or MOD. OP=MOD is default and implies that thermal load in different nodes is accumulated over all steps starting from the last perturbation step. Specifying the temperature for a node for which a temperature was defined in a previous step replaces this last value. OP=NEW implies that the temperatures are reinitialised to the initial values. If multiple *TEMPERATURE cards are present in a step this parameter takes effect for the first *TEMPERATURE card only.

For shell elements a temperature gradient can be defined in addition to a temperature. The temperature applies to nodes in the reference surface, the gradient acts in normal direction. For beam elements two gradients can be defined: one in 1-direction and one in 2-direction. Default for the gradients is zero.

The AMPLITUDE parameter allows for the specification of an amplitude by which the difference between the actual and initial temperature is scaled (mainly used for dynamic calculations). Thus, in that case the values entered on the *TEMPERATURE card are interpreted as reference values to be multiplied with the (time dependent) amplitude value to obtain the actual value. At the end of the step the reference value is replaced by the actual value at that time, for use in subsequent steps.

The TIME DELAY parameter modifies the AMPLITUDE parameter. As such, TIME DELAY must be preceded by an AMPLITUDE name. TIME DELAY is a time shift by which the AMPLITUDE definition it refers to is moved in positive time direction. For instance, a TIME DELAY of 10 means that for time t the amplitude is taken which applies to time t-10. The TIME DELAY parameter must only appear once on one and the same keyword card.

If the USER parameter is selected the temperature values are determined by calling the user subroutine utemp.f, which must be provided by the user. This applies to all nodes listed beneath the *TEMPERATURE keyword. Any temperature values specified behind the nodal numbers are not taken into account. If the USER parameter is selected, the AMPLITUDE parameter has no effect and should not be used.

The SUBMODEL parameter is used to specify that the nodes underneath the *TEMPERATURE card should get their temperature values by interpolation from a global model. Each of these nodes must be listed underneath exactly one nodal *SUBMODEL card. The SUBMODEL parameter automatically requires the use of the STEP parameter, specifying from which step in the global model the temperatures should be interpolated. If the SUBMODEL card is used no temperature values need be specified.

Temperature gradients are not influenced by the AMPLITUDE parameter.

First line:

- *TEMPERATURE

Following line:

- Node number or node set label.
- Temperature value at the node.
- Temperature gradient in normal direction (shells) or in 2-direction (beams).
- Temperature gradient in 1-direction (beams).

Repeat this line if needed.

```
Example:

*TEMPERATURE
N1,293.
300,473.
301,473.
302,473.
```

assigns a temperature T=293 to all nodes in (node) set N1, and T=473 to nodes 300, 301 and 302.

Example files: beam8t, beam20t, beamnlt, beamt4.

7.101 *TIE

Keyword type: model definition

This option is used to tie two surfaces. It can only be used with 3-dimensional elements (no plane stress, plane strain, axisymmetric, beam or shell elements).Optional parameters are POSITION TOLERANCE, NAME, CYCLIC SYMMETRY and MULTISTAGE. The dependent surface is called the slave surface, the independent surface is the master surface. The user can freely decide which surface is taken as slave and which as master. The surfaces are defined using *SURFACE. Nodes belonging to the dependent surface cannot be used as dependent nodes in other SPC's or MPC's. Only nodes on an axis of cyclic symmetry can belong to both the slave as well as to the master surface.

Default (i.e. in the absense of the CYCLIC SYMMETRY and the MULTISTAGE parameter) is a tie of two adjacent surfaces. This is also called tied contact. In that case MPC's are generated connecting the slave nodes with the master faces, provided the distance between the nodes and the adjacent face does not exceed the POSITION TOLERANCE. If no tolerance is specified, or the tolerance is smaller than 10^{-10}, a default tolerance is calculated equal to 2.5% of the typical element size. For tied contact the slave surface can be a nodal or element face surface, whereas the master surface has to consist of element faces. Nodes which are not connected are stored in file WarnNodeMissMasterIntersect.nam and can be read into CalculiX GraphiX by using the command "read WarnNodeMissMasterIntersect.nam inp". In order to create the MPC's connecting the slave and master side, the latter is triangulated. The triangulation is stored in file TriMasterContactTie.frd and can be visualized using CalculiX GraphiX.

The parameter CYCLIC SYMMETRY is used to tie two surfaces bounding one and the same datum sector in circumferential direction. Both the slave and the master surface can be node or face based. For face based surfaces the nodes belonging to the face are identied at the start of the algorithm which generates the cyclic multiple point constraints. For each slave node, a master node is determined which matches the slave node within a tolerance specified by the parameter POSITION TOLERANCE after rotation about the cyclic

symmetry axis . Subsequently, a cyclic symmetry constraint is generated. If no tolerance is specified, or the tolerance is smaller than 10^{-30}, a default tolerance is calculated equal to 0.5% of the mean of the distance of the master nodes to their closest neighbor. If no master node is found within the tolerance, the face on the master surface is identified to which the rotated slave node belongs, and a more elaborate multiple point constraint is generated. If none is found, the closest face is taken. If this face does not lie within 10% of its length from the slave node, an error is issued and the program stops.

The parameter MULTISTAGE is used to tie two coincident nodal surfaces (no face based surfaces allowed) each of which belongs to a different datum sector. In that way two axially neighboring datum sectors can be tied. In this case, the order in which the user specifies the surfaces is not relevant: the surface belonging to the smallest datum sector is taken as master surface. The larger datum sector should not extend the smaller datum sector by more than once the smaller datum sector, no matter in what circumferential direction (clockwise or counterclockwise). This option should not be used in the presence of network elements.

The parameter NAME is needed if more than one *TIE constraint is defined. It allows the user to distinguish the tie constraints when referring to them in other keyword cards (e.g. *CYCLIC SYMMETRY MODEL).

First line:

- *TIE
- enter the required parameter CYCLIC SYMMETRY and any of the optional parameters, if needed.

Following line:

- Name of the slave surface.
- Name of the master surface.

Example:

```
*TIE,POSITION TOLERANCE=0.01
left,right
```

defines a datum sector with slave surface left and master surface right, and defines a position tolerance of 0.01 length units.

Example files: segment, fullseg.

7.102 *TIME POINTS

Keyword type: model definition

This option may be used to specify a sequence of time points. If the parameter TIME=TOTAL TIME is used the reference time is the total time

since the start of the calculation, else it is the local step time. The parameter NAME, specifying a name for the time point sequence so that it can be referenced by output definitions (*NODE FILE, *EL FILE, *NODE PRINT or *EL PRINT) is required (maximum 80 characters).This option makes sense for nonlinear static, nonlinear dynamic, modal dynamic, heat transfer and coupled temperature-displacement calculations only. In all other procedures, this card is ignored.

In each step, the local step time starts at zero. Its upper limit is given by the time period of the step. This time period is specified on the *STATIC, *DYNAMIC, *HEAT TRANSFER or *COUPLED TEMPERATURE-DISPLACEMENT keyword card. The default step time period is 1.

The total time is the time accumulated until the beginning of the actual step augmented by the local step time.

GENERATE is the second optional parameter. If specified, the user can define a regular pattern of time points by specifying the starting time, the end time and the time increment.

First line:

- *TIME POINTS
- Enter the required parameter NAME, and the optional parameter if needed.

Following line, using as many entries as needed, if GENERATE is not specified:

- Time.
- Time.
- Time.
- Time.
- Time.
- Time.
- Time.
- Time.

Repeat this line if more than eight entries are needed.

Following line, using as many entries as needed, if GENERATE is specified:

- Starting time
- End time
- Time increment

Repeat this line if more than one regular sequence is needed.

```
Example:

*TIME POINTS,NAME=T1
.2,.3.,.8
```

defines a time points sequence with name T1 consisting of times .2, .3 and .8 time units. The time used is the local step time.

```
Example:

*TIME POINTS,NAME=T1,GENERATE
0.,3.,1.
```

defines a time points sequence with name T1 consisting of the time points 0., 1., 2., and 3. The time used is the local step time.

Example files: beamnlptp

7.103 *TRANSFORM

Keyword type: model definition

This option may be used to specify a local axis system X'-Y'-Z' to be used for defining SPC's, MPC's and nodal forces. For now, rectangular and cylindrical systems can be defined, triggered by the parameter TYPE=R (default) and TYPE=C.

A rectangular system is defined by specifying a point a on the local X' axis and a point b belonging to the X'-Y' plane but not on the X' axis. A right hand system is assumed (Figure 132).

When using a cylindrical system two points a and b on the axis must be given. The X' axis is in radial direction, the Z' axis in axial direction from point a to point b, and Y' is in tangential direction such that X'-Y'-Z' is a right hand system (Figure 133).

The parameter NSET, specifying the node set for which the transformation applies, is required.

If several transformations are defined for one and the same node, the last transformation takes effect.

Notice that a non-rectangular local coordinate system is not allowed in nodes which belong to plane stress, plane strain, or axisymmetric elements. If a local rectangular system is defined the local z-axis must coincide with the global z-axis (= axis orthogonal to the plane in which these elements are defined).

First line:

- *TRANSFORM
- Enter the required parameter NSET, and the optional parameter TYPE if needed.

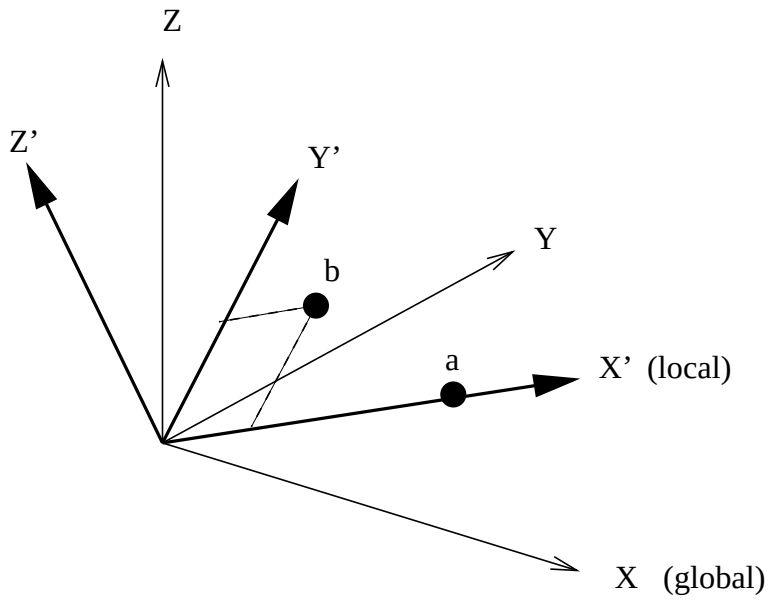


Figure 132: Definition of a rectangular coordinate system

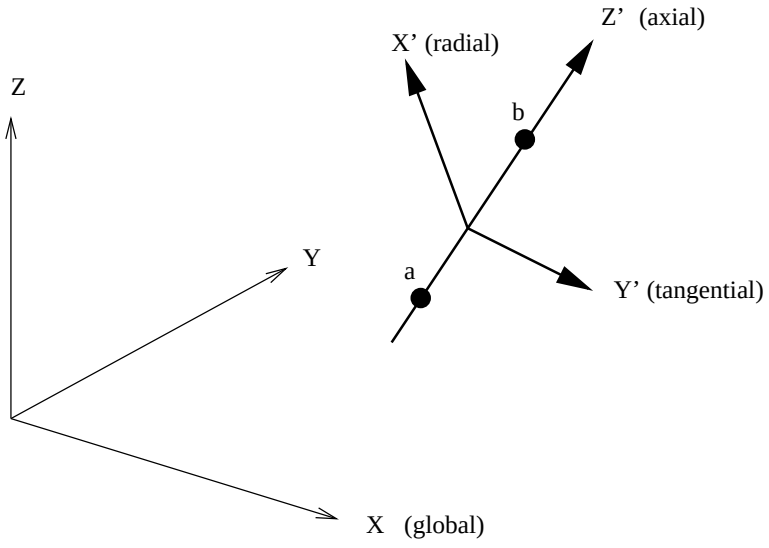


Figure 133: Definition of a cylindrical coordinate system

Second line:

- X-coordinate of point a.
- Y-coordinate of point a.
- Z-coordinate of point a.
- X-coordinate of point b.
- Y-coordinate of point b.
- Z-coordinate of point b.

Example:

```
*TRANSFORM,NSET=No1,TYPE=R
0.,1.,0.,0.,0.,1.
```

assigns a new rectangular coordinate system to the nodes belonging to (node) set No1. The x- and the y-axes in the local system are the y- and z-axes in the global system.

Example files: segment1, segment2, segmentf, segmentm.

7.104 *TRANSFORMF

Keyword type: model definition

This option may be used to specify a local axis system X'-Y'-Z' to be used for defining SPC's in CFD-calculations. For now, rectangular and cylindrical systems can be defined, triggered by the parameter TYPE=R (default) and TYPE=C.

A rectangular system is defined by specifying a point a on the local X' axis and a point b belonging to the X'-Y' plane but not on the X' axis. A right hand system is assumed (Figure 132).

When using a cylindrical system two points a and b on the axis must be given. The X' axis is in radial direction, the Z' axis in axial direction from point a to point b, and Y' is in tangential direction such that X'-Y'-Z' is a right hand system (Figure 133).

The difference with the *TRANSFORM card is that for CFD-calculations the SPC's are applied to element faces instead of nodes. The parameter SURFACE, specifying the surface for which the transformation applies, is required. Notice that this surface must be face-based.

First line:

- *TRANSFORM
- Enter the required parameter SURFACE, and the optional parameter TYPE if needed.

Second line:

- X-coordinate of point a.
- Y-coordinate of point a.
- Z-coordinate of point a.
- X-coordinate of point b.
- Y-coordinate of point b.
- Z-coordinate of point b.

Example:

```
*TRANSFORMF,SURFACE=ABC,TYPE=C
0.,0.,0.,1.,0.,0.
```

assigns a new cylindrical coordinate system to the faces belonging to surface ABC. The cylindrical axis is the global x-axis.

Example files: .

7.105 *UNCOUPLED TEMPERATURE-DISPLACEMENT

Keyword type: step

This procedure is used to perform an uncoupled thermomechanical analysis. For each increment a thermal analysis is performed first. Then, the resulting temperature field is used as boundary condition for a subsequent mechanical analysis for the same increment. Consequently, there is no feedback from the mechanical deformation on the temperature field within one and the same increment. Due to the sequential calculations the resulting systems of equations are smaller and faster execution times can be expected. Moreover, the number of iterations within the increment is determined for the thermal and mechanical analysis separately, whereas in a coupled thermomechanical analysis the worst convergent analysis dictates the number of iterations for

There are eight optional parameters: SOLVER, DIRECT, ALPHA, STEADY STATE, DELTMX, EXPLICIT, TIME RESET and TOTAL TIME AT START.

SOLVER determines the package used to solve the ensuing system of equations. The following solvers can be selected:

- the SGI solver
- PARDISO
- SPOOLES [3, 4].
- TAUCS

- the iterative solver by Rank and Ruecker [60], which is based on the algorithms by Schwarz [64].

Default is the first solver which has been installed of the following list: SGI, PARDISO, SPOOLES and TAUCS. If none is installed, the default is the iterative solver, which comes with the CalculiX package.

The SGI solver is the fastest, but is is proprietary: if you own SGI hardware you might have gotten the scientific software package as well, which contains the SGI sparse system solver. SPOOLES is also very fast, but has no out-of-core capability: the size of systems you can solve is limited by your RAM memory. With 2GB of RAM you can solve up to 250,000 equations. TAUCS is also good, but my experience is limited to the LL^T decomposition, which only applies to positive definite systems. It has an out-of-core capability and also offers a LU decomposition, however, I was not able to run either of them so far. Next comes the iterative solver. If SOLVER=ITERATIVE SCALING is selected, the preconditioning is limited to a scaling of the diagonal terms, SOLVER=ITERATIVE CHOLESKY triggers Incomplete Cholesky preconditioning. Cholesky preconditioning leads to a better convergence and maybe to shorter execution times, however, it requires additional storage roughly corresponding to the nonzeros in the matrix. If you are short of memory, diagonal scaling might be your last resort. The iterative methods perform well for truly three-dimensional structures. For instance, calculations for a hemisphere were about nine times faster with the ITERATIVE SCALING solver, and three times faster with the ITERATIVE CHOLESKY solver than with SPOOLES. For two-dimensional structures such as plates or shells, the performance might break down drastically and convergence often requires the use of Cholesky preconditioning. SPOOLES (and any of the other direct solvers) performs well in most situations with emphasis on slender structures but requires much more storage than the iterative solver. PARDISO is the Intel proprietary solver.

The parameter DIRECT indicates that automatic incrementation should be switched off. The increments will have the fixed length specified by the user on the second line.

The parameter ALPHA takes an argument between -1/3 and 0. It controls the dissipation of the high frequency responce: lower numbers lead to increased numerical damping ([53]). The default value is -0.05.

The parameter STEADY STATE indicates that only the steady state should be calculated. If this parameter is absent, the calculation is assumed to be time dependent and a transient analysis is performed. For a transient analysis the specific heat of the materials involved must be provided.

The parameter DELTMX can be used to limit the temperature change in two subsequent increments. If the temperature change exceeds DELTMX the increment is restarted with a size equal to D_A times DELTMX divided by the temperature change. The default for D_A is 0.85, however, it can be changed by the *CONTROLS keyword. DELTMX is only active in transient calculations. Default value is 10^{30}.

The parameter EXPLICIT is only important for fluid computations. If

present, the fluid computation is explicit, else it is semi-implicit. Coupled structural computations are always implicit.

The parameter TIME RESET can be used to force the total time at the end of the present step to coincide with the total time at the end of the previous step. If there is no previous step the targeted total time is zero. If this parameter is absent the total time at the end of the present step is the total time at the end of the previous step plus the time period of the present step (2nd parameter underneath the *UNCOUPLED TEMPERATURE-DISPLACEMENT keyword). Consequently, if the time at the end of the previous step is 10. and the present time period is 1., the total time at the end of the present step is 11. If the TIME RESET parameter is used, the total time at the beginning of the present step is 9. and at the end of the present step it will be 10. This is sometimes useful if transient uncoupled temperature-displacement calculations are preceded by a stationary heat transfer step to reach steady state conditions at the start of the transient uncoupled temperature-displacement calculations. Using the TIME RESET parameter in the stationary step (the first step in the calculation) will lead to a zero total time at the start of the subsequent instationary step.

Finally, the parameter TOTAL TIME AT START can be used to set the total time at the start of the step to a specific value.

First line:

- *UNCOUPLED TEMPERATURE-DISPLACEMENT
- Enter any needed parameters and their values.
- Initial time increment. This value will be modified due to automatic incrementation, unless the parameter DIRECT was specified (default 1.).
- Time period of the step (default 1.).
- Minimum time increment allowed. Only active if DIRECT is not specified. Default is the initial time increment or 1.e-5 times the time period of the step, whichever is smaller.
- Maximum time increment allowed. Only active if DIRECT is not specified. Default is 1.e+30.

Example:

```
*UNCOUPLED TEMPERATURE-DISPLACEMENT
.1,1.
```

defines an uncoupled thermomechanical step and selects the SPOOLES solver as linear equation solver in the step (default). The second line indicates that the initial time increment is .1 and the total step time is 1.

Example files: thermomech2.

7.106 *USER MATERIAL

Keyword type: model definition, material

This option is used to define the properties of a user-defined material. For a user-defined material a material subroutine has to be provided, see Sections 8.5 and 8.6. There is one required parameter CONSTANTS and one optional parameter TYPE.

The value of CONSTANTS indicates how many material constants are to be defined for this type of material. Right now, there is an upper limit of 21 constants for mechanical user-defined materials and 6 for thermal user-defined materials. If you need more, incorporate them in your user subroutine, change the source code, or contact the author to do so.

The parameter TYPE can take the value MECHANICAL or THERMAL. If TYPE=MECHANICAL the user routine characterizes the mechanical behavior of the material, i.e. the stress-strain behavior. This property is only important for mechanical or coupled temperature-displacement calculations. If TYPE=THERMAL the user routine defines the thermal behavior of the material, i.e. the heat flux versus temperature gradient behavior. This is only used in thermal or coupled temperature-displacement calculations. Default is TYPE=MECHANICAL.

The material is identified by means of the NAME parameter on the *MATERIAL card.

First line:

- *USER MATERIAL
- Enter the CONSTANTS parameter and its value

Give on the following int(CONSTANTS/8)+1 lines the constants followed by the temperature value for which they are valid, 8 values per line. The value of the temperature can be left blank, however, if CONSTANTS is a multiple of 8 a blank line must be provided if the temperature is left blank. Repeat the set of constants if values for more than one temperature are given.

Example:

```
*USER MATERIAL,CONSTANTS=8
500000.,157200.,400000.,157200.,157200.,300000.,126200.,126200.,
294.
300000.,57200.,300000.,57200.,57200.,200000.,26200.,26200.,
394.
```

defines a user-defined material with eight constants for two different temperatures, 294 and 394.

Example files: beamu.

7.107 *VALUES AT INFINITY

Keyword type: model definition

This keyword is used to define values at infinity for 3D fluid calculations. They are used to calculate the pressure coefficient c_P if requested as output by the user (*NODE FILE) and freestream boundary conditions for the turbulence parameters [48].

First line:

- *VALUES AT INFINITY

Second line:

- Static temperature at infinity
- Norm of the velocity vector at infinity
- Static pressure at infinity
- Density at infinity
- Length of the computational domain

```
Example:

*VALUES AT INFINITY
40.,1.,11.428571,1.,40.
```

specifies a static temperature of 40., a velocity of 1., a static pressure of 11.428571 and a density of 1. at infinity. The size of the computational domain is 40.

Example files: fluid1,fluid2.

7.108 *VIEWFACTOR

Keyword type: step

Sometimes you wish to reuse the viewfactors calculated in a previous run, or store the present viewfactors to file for future use. This can be done using the keyword card *VIEWFACTOR.

There are six optional parameters: READ, WRITE, WRITE ONLY, NO CHANGE, INPUT and OUTPUT. READ/NO CHANGE and WRITE/WRITE ONLY are mutually exclusive, i.e. if you specify READ you cannot specify WRITE or WRITE ONLY and so on. These parameters are used to specify whether you want to read previous viewfactors (READ/NO CHANGE) or store the viewfactors of the present calculation for future runs (WRITE and WRITE ONLY). For reading there is an optional parameter INPUT, for writing there is an optional parameter OUTPUT.

If you specify READ or NO CHANGE, the results will be read from the binary file "jobname.vwf" (which should have been generated in a previous run) unless you use the parameter INPUT. In the latter case you can specify any filename (maximum 126 characters) containing the viewfactors. If the filename contains blanks, it must be delimited by double quotes and the filename should not exceed 124 characters. The geometry of the faces exchanging radiation must be exactly the same as in the actual run. Notice that the parameter INPUT must be preceded by the READ or NO CHANGE parameter. The parameter NO CHANGE has the same effect as the READ parameter except that it additionally specifies that the viewfactors did not change compared with the previous step. If this parameter is selected the LU decomposition of the radiation matrix is not repeated and a lot of computational time can be saved. This parameter can obviously not be used in the first step of the calculation.

In thermal calculations (keyword *HEAT TRANSFER) the viewfactors are calculated at the start of each step since the user can change the radiation boundary conditions in each step. If the viewfactors are not read from file, i.e. if there is no *VIEWFACTOR,READ or *VIEWFACTOR,NO CHANGE card in a step they are calculated from scratch. In thermomechanical calculations (keyword *COUPLED TEMPERATURE-DISPLACEMENT) the viewfactors are calculated at the start of each iteration. Indeed, the deformation of the structure in the previous iteration can lead to a change of the viewfactors. However, if the user reads the viewfactors from file the recalculation of the viewfactors in each iteration anew is turned off. In that case it is assumed that the viewfactors do not change during the entire step.

If you specify WRITE or WRITE ONLY, the viewfactors will be stored in binary format in file "jobname.vwf" unless you use the parameter OUTPUT. In the latter case you can specify any filename (maximum 125 characters) in which the viewfactors are to be written. Any existing file with this name will be deleted prior to the writing operation. If the filename contains blanks, it must be delimited by double quotes and the filename should not exceed 123 characters. Notice that the parameter OUTPUT must be preceded by the WRITE or WRITE ONLY parameter. If you specify WRITE ONLY the program stops after calculating and storing the viewfactors.

A *VIEWFACTOR card is only active in the step in which it occurs.

First and only line:

- *VIEWFACTOR
- specify either READ or WRITE

Example:

```
*VIEWFACTOR,WRITE
```

will store the viewfactors calculated in that step to file.

```
Example:

*VIEWFACTOR,READ,INPUT=viewfactors.dat
```

will read the viewfactors from file viewfactors.dat.

Example files: furnace.

7.109 *VISCO

Keyword type: step

This procedure is used to perform a static analysis for materials with viscous behavior. The syntax is identical to the *STATIC syntax. Notice that the default way of applying loads in a *VISCO step is step loading, i.e. the loading is fully applied at the start of the step. This is different from a *STATIC step, in which the loading is ramped. Using a *VISCO step only makes sense if at least one materials exhibits viscous behavior.

8 User subroutines.

Although the present software is protected by the GNU General Public License, and the user should always get the source code, it is sometimes more practical to get a nicely described user interface to plug in your own routines, instead of having to analyze the whole program. Therefore, for specific tasks well-defined interfaces are put at the disposal of the user. These interfaces are basically FORTRAN subroutines containing a subroutine header, a description of the input and output variables and declaration statements for these variables. The body of the routine has to be written by the user.

8.1 Creep (creep.f)

The user subroutine "creep.f" is made available to allow the user to incorporate his own creep law by selecting the keyword sequence *CREEP,LAW=USER in the input deck. The input/output depends on the kind of material: if the elastic properties of the material are isotropic, the Von Mises stress goes in and the equivalent deviatoric creep strain increment and its derivative with respect to the Von Mises stress for a given Von Mises stress come out. If the elastic properties of the material are anisotropic, the equivalent deviatoric creep strain increment goes in and the Von Mises stress and the derivative of the equivalent deviatoric creep strain increment with respect to the Von Mises stress come out. The creep regime is, however, always isotropic. Whether the elastic regime is isotropic or anisotropic is triggered by the value of the variable lend.The header and a description of the input and output variables is as follows:

```
      subroutine creep(decra,deswa,statev,serd,ec,esw,p,qtild,
```

```
     &  temp,dtemp,predef,dpred,time,dtime,cmname,leximp,lend,
     &  coords,nstatv,noel,npt,layer,kspt,kstep,kinc)
!
!     user creep routine
!
!     INPUT (general):
!
!     statev(1..nstatv)  internal variables
!     serd               not used
!     ec(1)              equivalent creep at the start of the increment
!     ec(2)              not used
!     esw(1..2)          not used
!     p                  not used
!     temp               temperature at the end of the increment
!     dtemp              not used
!     predef             not used
!     dpred              not used
!     time(1)            value of the step time at the end of the increment
!     time(2)            value of the total time at the end of the increment
!     dtime              time increment
!     cmname             material name
!     leximp             not used
!     lend               if = 2: isotropic creep
!                        if = 3: anisotropic creep
!     coords(1..3)       coordinates of the current integration point
!     nstatv             number of internal variables
!     noel               element number
!     npt                integration point number
!     layer              not used
!     kspt               not used
!     kstep              not used
!     kinc               not used
!
!    INPUT only for elastic isotropic materials:
!     qtild              von Mises stress
!
!    INPUT only for elastic anisotropic materials:
!     decra(1)           equivalent deviatoric creep strain increment
!
!
!     OUTPUT (general):
!
!     decra(1)           equivalent deviatoric creep strain increment
!     decra(2..4)        not used
!     decra(5)           derivative of the equivalent deviatoric
!                        creep strain increment w.r.t. the von Mises
```

```
!                       stress
!     deswa(1..5)       not used
!
!     OUTPUT only for elastic isotropic materials:
!     decra(1)          equivalent deviatoric creep strain increment
!
!     OUTPUT only for elastic anisotropic materials:
!     qtild             von Mises stress
!
```

8.2 Hardening (uhardening.f)

In subroutine "uhardening.f", the user can insert his own isotropic and/or kinematic hardening laws for (visco)plastic behavior governed by the keyword sequence *PLASTIC,HARDENING=USER. The header and variable description is as follows:

```
      subroutine uhardening(amat,iel,iint,t1l,epini,ep,dtime,fiso,dfiso,
     &                      fkin,dfkin)
!
!     INPUT:
!
!     amat:    material name (maximum 80 characters)
!     iel:     element number
!     iint:    integration point number
!     t1l:     temperature at the end of the increment
!     epini:   equivalent irreversible strain at the start
!              of the increment
!     ep:      present equivalent irreversible strain
!     dtime:   time increment
!
!     OUTPUT:
!
!     fiso:    present isotropic hardening Von Mises stress
!     dfiso:   present isotropic hardening tangent (derivative
!              of the Von Mises stress with respect to the
!              equivalent irreversible strain)
!     fkin:    present kinematic hardening Von Mises stress
!     dfkin:   present kinematic hardening tangent (derivative
!              of the Von Mises stress with respect to the
!              equivalent irreversible strain)
!
```

8.3 User-defined initial conditions

These routines are an alternative to the explicit inclusion of the initial conditions underneath the *INITIAL CONDITIONS keyword card in the input deck. They allow for a more flexible definition of initial conditions.

8.3.1 Initial internal variables (sdvini.f)

This subroutine is used for user-defined internal variables, characterized by the parameter USER on the *INITIAL CONDITIONS,TYPE=SOLUTION card. The header and variable description is as follows:

```
      subroutine sdvini(statev,coords,nstatv,ncrds,noel,npt,
     &  layer,kspt)
!
!     user subroutine sdvini
!
!
!     INPUT:
!
!     coords(1..3)       global coordinates of the integration point
!     nstatv             number of internal variables (must be
!                        defined by the user with the *DEPVAR card)
!     ncrds              number of coordinates
!     noel               element number
!     npt                integration point number
!     layer              not used
!     kspt               not used
!
!     OUTPUT:
!
!     statev(1..nstatv)  initial value of the internal state
!                        variables
```

8.3.2 Initial stress field (sigini.f)

This subroutine is used for user-defined initial stresses, characterized by the parameter USER on the *INITIAL CONDITIONS,TYPE=STRESS card. The header and variable description is as follows:

```
      subroutine sigini(sigma,coords,ntens,ncrds,noel,npt,layer,
     &  kspt,lrebar,rebarn)
!
!     user subroutine sigini
!
!     INPUT:
!
```

```
!     coords             coordinates of the integration point
!     ntens              number of stresses to be defined
!     ncrds              number of coordinates
!     noel               element number
!     npt                integration point number
!     layer              currently not used
!     kspt               currently not used
!     lrebar             currently not used (value: 0)
!     rebarn             currently not used
!
!     OUTPUT:
!
!     sigma(1..ntens)    initial stress values in the integration
!                        point. If ntens=6 the order of the
!                        components is 11,22,33,12,13,23
!
```

8.4 User-defined loading

These routines are made available to define nonuniform distributed loading. The user can define the loading in each integration point separately as a function of position, time etc.

8.4.1 Concentrated flux (cflux.f)

This subroutine is used for user-defined concentrated heat flux, characterized by the parameter USER on the *CFLUX card. The header and variable description is as follows:

```
      subroutine cflux(flux,msecpt,kstep,kinc,time,node,coords,vold,
     &  mi)
!
!     user subroutine cflux
!
!
!     INPUT:
!
!     msecpt             number of flux values (for volume elements:1)
!     kstep              step number
!     kinc               increment number
!     time(1)            current step time
!     time(2)            current total time
!     node               node number
!     coords(1..3)       global coordinates of the node
!     vold(0..4,1..nk)   solution field in all nodes
!                        0: temperature
```

```
!                       1: displacement in global x-direction
!                       2: displacement in global y-direction
!                       3: displacement in global z-direction
!                       4: static pressure
!     mi(1)             max # of integration points per element (max
!                       over all elements)
!     mi(2)             max degree of freedom per node (max over all
!                       nodes) in fields like v(0:mi(2))...
!
!     OUTPUT:
!
!     flux(1..msecpt)   concentrated flux in the node
!
```

8.4.2 Concentrated load (cload.f)

This subroutine is used for user-defined concentrated load, characterized by the parameter USER on the *CLOAD card. The header and variable description is as follows:

```
      subroutine cload(xload,kstep,kinc,time,node,idof,coords,vold,
     &  mi,ntrans,trab,inotr,veold)
!
!     user subroutine cload
!
!
!     INPUT:
!
!     kstep             step number
!     kinc              increment number
!     time(1)           current step time
!     time(2)           current total time
!     node              node number
!     idof              degree of freedom
!     coords(1..3)      global coordinates of the node
!     vold(0..mi(2)
!              ,1..nk)  solution field in all nodes (for modal
!                       dynamics: in all nodes for which output
!                       was requested or a force was applied)
!                       0: temperature
!                       1: displacement in global x-direction
!                       2: displacement in global y-direction
!                       3: displacement in global z-direction
!                       4: static pressure
!     mi(1)             max # of integration points per element (max
!                       over all elements)
```

```
!     mi(2)              max degree of freedomm per node (max over all
!                        nodes) in fields like v(0:mi(2))...
!     veold(0..3,1..nk)  derivative of the solution field w.r.t.
!                        time in all nodes(for modal
!                        dynamics: in all nodes for which output
!                        was requested or a force was applied)
!                        0: temperature rate
!                        1: velocity in global x-direction
!                        2: velocity in global y-direction
!                        3: velocity in global z-direction
!     ntrans             number of transform definitions
!     trab(1..6,i)       coordinates of two points defining transform i
!     trab(7,i)          -1: cylindrical transformation
!                         1: rectangular transformation
!     inotr(1,j)         transformation number applied to node j
!     inotr(2,j)         a SPC in a node j in which a transformation
!                        applied corresponds to a MPC. inotr(2,j)
!                        contains the number of a new node generated
!                        for the inhomogeneous part of the MPC
!
!     OUTPUT:
!
!     xload              concentrated load in direction idof of node
!                        "node" (global coordinates)
!
```

8.4.3 Distributed flux (dflux.f)

This subroutine is used for nonuniform heat flux, characterized by distributed load labels of the form SxNUy, cf *DFLUX. The load label can be up to 20 characters long. In particular, y can be used to distinguish different nonuniform flux patterns. The header and variable description is as follows:

```
      subroutine dflux(flux,sol,kstep,kinc,time,noel,npt,coords,
     &     jltyp,temp,press,loadtype,area,vold,co,lakonl,konl,
     &     ipompc,nodempc,coefmpc,nmpc,ikmpc,ilmpc,iscale,mi)
!
!     user subroutine dflux
!
!
!     INPUT:
!
!     sol                current temperature value
!     kstep              step number
!     kinc               increment number
!     time(1)            current step time
```

```
!     time(2)            current total time
!     noel               element number
!     npt                integration point number
!     coords(1..3)       global coordinates of the integration point
!     jltyp              loading face kode:
!                        1  = body flux
!                        11 = face 1
!                        12 = face 2
!                        13 = face 3
!                        14 = face 4
!                        15 = face 5
!                        16 = face 6
!     temp               currently not used
!     press              currently not used
!     loadtype           load type label
!     area               for surface flux: area covered by the
!                            integration point
!                        for body flux: volume covered by the
!                            integration point
!     vold(0..4,1..nk)   solution field in all nodes
!                        0: temperature
!                        1: displacement in global x-direction
!                        2: displacement in global y-direction
!                        3: displacement in global z-direction
!                        4: static pressure
!     co(3,1..nk)        coordinates of all nodes
!                        1: coordinate in global x-direction
!                        2: coordinate in global y-direction
!                        3: coordinate in global z-direction
!     lakonl             element label
!     konl(1..20)        nodes belonging to the element
!     ipompc(1..nmpc))   ipompc(i) points to the first term of
!                        MPC i in field nodempc
!     nodempc(1,*)       node number of a MPC term
!     nodempc(2,*)       coordinate direction of a MPC term
!     nodempc(3,*)       if not 0: points towards the next term
!                                  of the MPC in field nodempc
!                        if 0: MPC definition is finished
!     coefmpc(*)         coefficient of a MPC term
!     nmpc               number of MPC's
!     ikmpc(1..nmpc)     ordered global degrees of freedom of the MPC's
!                        the global degree of freedom is
!                        8*(node-1)+direction of the dependent term of
!                        the MPC (direction = 0: temperature;
!                        1-3: displacements; 4: static pressure;
!                        5-7: rotations)
```

```
!     ilmpc(1..nmpc)     ilmpc(i) is the MPC number corresponding
!                        to the reference number in ikmpc(i)
!     mi(1)              max # of integration points per element (max
!                        over all elements)
!     mi(2)              max degree of freedomm per node (max over all
!                        nodes) in fields like v(0:mi(2))...
!
!     OUTPUT:
!
!     flux(1)            magnitude of the flux
!     flux(2)            not used; please do NOT assign any value
!     iscale             determines whether the flux has to be
!                        scaled for increments smaller than the
!                        step time in static calculations
!                        0: no scaling
!                        1: scaling (default)
!
```

8.4.4 Distribruted load (dload.f)

This subroutine is used for nonuniform pressure, characterized by distributed load labels of the form PxNUy, cf *DLOAD. The load label can be up to 20 characters long. In particular, y can be used to distinguish different nonuniform loading patterns. The header and variable description is as follows:

```
      subroutine dload(f,kstep,kinc,time,noel,npt,layer,kspt,
     &     coords,jltyp,loadtype,vold,co,lakonl,konl,
     &     ipompc,nodempc,coefmpc,nmpc,ikmpc,ilmpc,iscale,veold,
     &     rho,amat,mi)
!
!     user subroutine dload
!
!
!     INPUT:
!
!     kstep              step number
!     kinc               increment number
!     time(1)            current step time
!     time(2)            current total time
!     noel               element number
!     npt                integration point number
!     layer              currently not used
!     kspt               currently not used
!     coords(1..3)       global coordinates of the integration point
!     jltyp              loading face kode:
!                        21 = face 1
```

```
!                       22 = face 2
!                       23 = face 3
!                       24 = face 4
!                       25 = face 5
!                       26 = face 6
!     loadtype          load type label
!     vold(0..4,1..nk)  solution field in all nodes
!                       0: temperature
!                       1: displacement in global x-direction
!                       2: displacement in global y-direction
!                       3: displacement in global z-direction
!                       4: static pressure
!     veold(0..3,1..nk) derivative of the solution field w.r.t.
!                       time in all nodes
!                       0: temperature rate
!                       1: velocity in global x-direction
!                       2: velocity in global y-direction
!                       3: velocity in global z-direction
!     co(3,1..nk)       coordinates of all nodes
!                       1: coordinate in global x-direction
!                       2: coordinate in global y-direction
!                       3: coordinate in global z-direction
!     lakonl            element label
!     konl(1..20)       nodes belonging to the element
!     ipompc(1..nmpc))  ipompc(i) points to the first term of
!                       MPC i in field nodempc
!     nodempc(1,*)      node number of a MPC term
!     nodempc(2,*)      coordinate direction of a MPC term
!     nodempc(3,*)      if not 0: points towards the next term
!                                 of the MPC in field nodempc
!                       if 0: MPC definition is finished
!     coefmpc(*)        coefficient of a MPC term
!     nmpc              number of MPC's
!     ikmpc(1..nmpc)    ordered global degrees of freedom of the MPC's
!                       the global degree of freedom is
!                       8*(node-1)+direction of the dependent term of
!                       the MPC (direction = 0: temperature;
!                       1-3: displacements; 4: static pressure;
!                       5-7: rotations)
!     ilmpc(1..nmpc)    ilmpc(i) is the MPC number corresponding
!                       to the reference number in ikmpc(i)
!     rho               local density
!     amat              material name
!     mi(1)             max # of integration points per element (max
!                       over all elements)
!     mi(2)             max degree of freedomm per node (max over all
```

```
!                       nodes) in fields like v(0:mi(2))...
!
!     OUTPUT:
!
!     f                 magnitude of the distributed load
!     iscale            determines whether the flux has to be
!                       scaled for increments smaller than the
!                       step time in static calculations
!                       0: no scaling
!                       1: scaling (default)
!
```

8.4.5 Heat convection (film.f)

This subroutine is used for nonuniform convective heat flux, characterized by distributed load labels of the form FxNUy, cf *FILM. The load label can be up to 20 characters long. In particular, y can be used to distinguish different nonuniform film patterns. The header and variable description is as follows:

```
      subroutine film(h,sink,temp,kstep,kinc,time,noel,npt,
     &  coords,jltyp,field,nfield,loadtype,node,area,vold,mi)
!
!     user subroutine film
!
!
!     INPUT:
!
!     sink              most recent sink temperature
!     temp              current temperature value
!     kstep             step number
!     kinc              increment number
!     time(1)           current step time
!     time(2)           current total time
!     noel              element number
!     npt               integration point number
!     coords(1..3)      global coordinates of the integration point
!     jltyp             loading face kode:
!                       11 = face 1
!                       12 = face 2
!                       13 = face 3
!                       14 = face 4
!                       15 = face 5
!                       16 = face 6
!     field             currently not used
!     nfield            currently not used (value = 1)
!     loadtype          load type label
```

```
!     node               network node (only for forced convection)
!     area               area covered by the integration point
!     vold(0..4,1..nk)   solution field in all nodes
!                        0: temperature
!                        1: displacement in global x-direction
!                        2: displacement in global y-direction
!                        3: displacement in global z-direction
!                        4: static pressure
!     mi(1)              max # of integration points per element (max
!                        over all elements)
!     mi(2)              max degree of freedomm per node (max over all
!                        nodes) in fields like v(0:mi(2))...
!
!     OUTPUT:
!
!     h(1)               magnitude of the film coefficient
!     h(2)               not used; please do NOT assign any value
!     sink               (updated) sink temperature (need not be
!                        defined for forced convection)
!
```

8.4.6 Boundary conditions(uboun.f)

This subroutine is used for user-defined boundary values, characterized by the parameter USER on the *BOUNDARY card. The header and variable description is as follows:

```
      subroutine uboun(boun,kstep,kinc,time,node,idof,coords,vold,mi)
!
!     user subroutine uboun
!
!
!     INPUT:
!
!     kstep              step number
!     kinc               increment number
!     time(1)            current step time
!     time(2)            current total time
!     node               node number
!     idof               degree of freedom
!     coords  (1..3)     global coordinates of the node
!     vold(0..4,1..nk)   solution field in all nodes
!                        0: temperature
!                        1: displacement in global x-direction
!                           (or mass flow rate for fluid nodes)
!                        2: displacement in global y-direction
```

```
!                       3: displacement in global z-direction
!                       4: static pressure
!     mi(1)             max # of integration points per element (max
!                       over all elements)
!     mi(2)             max degree of freedomm per node (max over all
!                       nodes) in fields like v(0:mi(2))...
!
!     OUTPUT:
!
!     boun              boundary value for degree of freedom idof
!                       in node "node"
!
```

8.4.7 Heat radiation (radiate.f)

This subroutine is used for nonuniform radiation heat flux, characterized by distributed load labels of the form RxNUy, cf *RADIATE. The load label can be up to 20 characters long. In particular, y can be used to distinguish different nonuniform radiation patterns. The header and variable description is as follows:

```
!
      subroutine radiate(e,sink,temp,kstep,kinc,time,noel,npt,
     &  coords,jltyp,field,nfield,loadtype,node,area,vold,mi,
     &  iemchange)
!
!     user subroutine radiate
!
!
!     INPUT:
!
!     sink              present sink temperature
!     temp              current temperature value
!     kstep             step number
!     kinc              increment number
!     time(1)           current step time
!     time(2)           current total time
!     noel              element number
!     npt               integration point number
!     coords(1..3)      global coordinates of the integration point
!     jltyp             loading face kode:
!                       11 = face 1
!                       12 = face 2
!                       13 = face 3
!                       14 = face 4
!                       15 = face 5
!                       16 = face 6
```

```
!     field              currently not used
!     nfield             currently not used (value = 1)
!     loadtype           load type label
!     node               currently not used
!     area               area covered by the integration point
!     vold(0..4,1..nk)   solution field in all nodes
!                        0: temperature
!                        1: displacement in global x-direction
!                        2: displacement in global y-direction
!                        3: displacement in global z-direction
!                        4: static pressure
!     mi(1)              max # of integration points per element (max
!                        over all elements)
!     mi(2)              max degree of freedomm per node (max over all
!                        nodes) in fields like v(0:mi(2))...
!
!     OUTPUT:
!
!     e(1)               magnitude of the emissivity
!     e(2)               not used; please do NOT assign any value
!     sink               sink temperature (need not be defined
!                        for cavity radiation)
!     iemchange          = 1 if the emissivity is changed during
!                        a step, else zero.
!
```

8.4.8 Temperature (utemp.f)

With this subroutine the user can define a temperature field. It is triggered bythe parameter USER on the *TEMPERATURE card. The header and variable description is as follows:

```
      subroutine utemp(temp,msecpt,kstep,kinc,time,node,coords,vold,
     &  mi)
!
!     user subroutine utemp
!
!
!     INPUT:
!
!     msecpt             number of temperature values (for volume elements:1)
!     kstep              step number
!     kinc               increment number
!     time(1)            current step time
!     time(2)            current total time
!     node               node number
```

```
!     coords(1..3)       global coordinates of the node
!     vold(0..4,1..nk)   solution field in all nodes
!                        0: temperature
!                        1: displacement in global x-direction
!                        2: displacement in global y-direction
!                        3: displacement in global z-direction
!                        4: static pressure
!     mi(1)              max # of integration points per element (max
!                        over all elements)
!     mi(2)              max degree of freedomm per node (max over all
!                        nodes) in fields like v(0:mi(2))...
!
!     OUTPUT:
!
!     temp(1..msecpt)    temperature in the node
!
```

8.4.9 Amplitude (uamplitude.f)

With this subroutine the user can define an amplitude. It is triggered bythe parameter USER on the *AMPLITUDE card. The header and variable description is as follows:

```
      subroutine uamplitude(time,name,amplitude)
!
!     user subroutine uamplitude: user defined amplitude definition
!
!     INPUT:
!
!     name               amplitude name
!     time               time at which the amplitude is to be
!                        evaluated
!
!     OUTPUT:
!
!     amplitude          value of the amplitude at time
!
```

8.4.10 Face loading (ufaceload.f)

This routine is called at the beginning of each step and can be used to determine the area of faces on which loading is applied. In that way the flux through the face can be calculated and stored in an extra file. This can be beneficial for thermal calculations to check the heat flux due to convection and radiation.

```
      subroutine ufaceload(co,ipkon,kon,lakon,
     &  nelemload,sideload,nload)
```

```
!
!
!     INPUT:
!
!     co(0..3,1..nk)     coordinates of the nodes
!     ipkon(*)           element topology pointer into field kon
!     kon(*)             topology vector of all elements
!     lakon(*)           vector with elements labels
!     nelemload(1..2,*)  1: elements faces of which are loaded
!                        2: nodes for environmental temperatures
!     sideload(*)        load label
!     nload              number of facial distributed loads
!
!     user routine called at the start of each step; possible use:
!     calculation of the area of sets of elements for
!     further use to calculate film or radiation coefficients.
!     The areas can be shared using common blocks.
!
```

8.4.11 Gap conductance (gapcon.f)

This subroutine is used to define the gap conductance across a contact pair (penalty contact only). cf *GAP CONDUCTANCE. The header and variable description is as follows:

```
      subroutine gapcon(ak,d,flowm,temp,predef,time,ciname,slname,
     &   msname,coords,noel,node,npred,kstep,kinc,area)
!
!     user subroutine gapcon
!
!
!     INPUT:
!
!     d(1)               separation between the surfaces
!     d(2)               pressure transmitted across the surfaces
!     flowm              not used
!     temp(1)            temperature at the slave node
!     temp(2)            temperature at the corresponding master
!                        position
!     predef             not used
!     time(1)            step time at the end of the increment
!     time(2)            total time at the end of the increment
!     ciname             surface interaction name
!     slname             not used
!     msname             not used
!     coords(1..3)       coordinates of the slave node
```

```
!     noel               element number of the contact spring element
!     node               slave node number
!     npred              not used
!     kstep              step number
!     kinc               increment number
!     area               slave area
!
!     OUTPUT:
!
!     ak(1)              gap conductance
!     ak(2..5)           not used
!
```

8.5 User-defined mechanical material laws.

This is an extremely important and powerful interface, allowing the user to define his/her own mechanical material behavior. The subroutine "umat.f" is a driver subroutine, calling user-defined routines similar to "umat_user.f", depending on the kind of material present in the model. To create a new material law, a "umat_user.f" routine must be written and an appropriate call must be inserted in routine "umat.f". In "umat.f" the name of the user material is to be defined. This is a character string the NAME parameter following the keyword card *MATERIAL has to start with. For instance, if you define a new material with the name FUNNY_MATERIAL, then in order to use this material, the material name has to start with this string. This is the main difference in usage between predefined and user-defined materials in CalculiX: if you use predefined materials you are completely free to choose a name for your material, if you use a user-defined material, its name has to start with a predefined string. Since a material name can be up to 80 characters long, there is generally enough freedom to define several versions of this material, e.g. FUNNY_MATERIAL1, FUNNY_MATERIAL2 etc.

The header and input/output variables of the umat_user routine are as follows:

```
      subroutine umat_user(amat,iel,iint,kode,elconloc,emec,emec0,
     &        beta,xokl,voj,xkl,vj,ithermal,t1l,dtime,time,ttime,
     &        icmd,ielas,mi,nstate_,xstateini,xstate,stre,stiff,
     &        iorien,pgauss,orab,pnewdt,ipkon)
!
!     calculates stiffness and stresses for a user defined material
!     law
!
!     icmd=3: calcutates stress at mechanical strain
!     else: calculates stress at mechanical strain and the stiffness
!           matrix
!
```

```
!     INPUT:
!
!     amat              material name
!     iel               element number
!     iint              integration point number
!
!     kode              material type (-100-#of constants entered
!                       under *USER MATERIAL): can be used for materials
!                       with varying number of constants
!
!     elconloc(21)      user defined constants defined by the keyword
!                       card *USER MATERIAL (max. 21, actual # =
!                       -kode-100), interpolated for the
!                       actual temperature t1l
!
!     emec(6)           Lagrange mechanical strain tensor (component order:
!                       11,22,33,12,13,23) at the end of the increment
!                       (thermal strains are subtracted)
!     emec0(6)          Lagrange mechanical strain tensor at the start of the
!                       increment (thermal strains are subtracted)
!     beta(6)           residual stress tensor (the stress entered under
!                       the keyword *INITIAL CONDITIONS,TYPE=STRESS)
!
!     xokl(3,3)         deformation gradient at the start of the increment
!     voj               Jacobian at the start of the increment
!     xkl(3,3)          deformation gradient at the end of the increment
!     vj                Jacobian at the end of the increment
!
!     ithermal          0: no thermal effects are taken into account
!                       >0: thermal effects are taken into account (triggered
!                       by the keyword *INITIAL CONDITIONS,TYPE=TEMPERATURE)
!     t1l               temperature at the end of the increment
!     dtime             time length of the increment
!     time              step time at the end of the current increment
!     ttime             total time at the start of the current step
!
!     icmd              not equal to 3: calculate stress and stiffness
!                       3: calculate only stress
!     ielas             0: no elastic iteration: irreversible effects
!                       are allowed
!                       1: elastic iteration, i.e. no irreversible
!                          deformation allowed
!
!     mi(1)             max. # of integration points per element in the
!                       model
!     nstate_           max. # of state variables in the model
```

```
!
!     xstateini(nstate_,mi(1),# of elements)
!                         state variables at the start of the increment
!     xstate(nstate_,mi(1),# of elements)
!                         state variables at the end of the increment
!
!     stre(6)             Piola-Kirchhoff stress of the second kind
!                         at the start of the increment
!
!     iorien              number of the local coordinate axis system
!                         in the integration point at stake (takes the value
!                         0 if no local system applies)
!     pgauss(3)           global coordinates of the integration point
!     orab(7,*)           description of all local coordinate systems.
!                         If a local coordinate system applies the global
!                         tensors can be obtained by premultiplying the local
!                         tensors with skl(3,3). skl is  determined by calling
!                         the subroutine transformatrix:
!                         call transformatrix(orab(1,iorien),pgauss,skl)
!
!
!     OUTPUT:
!
!     xstate(nstate_,mi(1),# of elements)
!                         updated state variables at the end of the increment
!     stre(6)             Piola-Kirchhoff stress of the second kind at the
!                         end of the increment
!     stiff(21):          consistent tangent stiffness matrix in the material
!                         frame of reference at the end of the increment. In
!                         other words: the derivative of the PK2 stress with
!                         respect to the Lagrangian strain tensor. The matrix
!                         is supposed to be symmetric, only the upper half is
!                         to be given in the same order as for a fully
!                         anisotropic elastic material (*ELASTIC,TYPE=ANISO).
!                         Notice that the matrix is an integral part of the
!                         fourth order material tensor, i.e. the Voigt notation
!                         is not used.
!     pnewdt              to be specified by the user if the material
!                         routine is unable to return the stiffness matrix
!                         and/or the stress due to divergence within the
!                         routine. pnewdt is the factor by which the time
!                         increment is to be multiplied in the next
!                         trial and should exceed zero but be less than 1.
!                         Default is -1 indicating that the user routine
!                         has converged.
!     ipkon(*)            ipkon(iel) points towards the position in field
```

```
!                       kon prior to the first node of the element's
!                       topology. If ipkon(iel) is smaller than 0, the
!                       element is not used.
```

The parameter ielas indicates whether irreversible effects should be taken into account. Forced displacements can lead to huge strains in the first iteration. Therefore, convergence in quasistatic calculations is often enhanced if the first iteration is completely linear, i.e. material and geometric nonlinearities are turned off. The parameter ielas is the appropriate flag.

Two extra routines are at the user's disposal for conversion purposes. "str2mat.f" can be used to convert Lagrangian strain into Eulerian strain, Cauchy stress into PK2 stress, or Kirchhoff stress into PK2 stress. The header and a short description are as follows:

```
      subroutine str2mat(str,ckl,vj,cauchy)
!
!     converts the stress in spatial coordinates into material coordinates
!     or the strain in material coordinates into spatial coordinates.
!
!     INPUT:
!
!     str(6):     Cauchy stress, Kirchhoff stress or Lagrange strain
!                 component order: 11,22,33,12,13,23
!     ckl(3,3):   the inverse deformation gradient
!     vj:         Jakobian determinant
!     cauchy:     logical variable
!                 if true: str contains the Cauchy stress
!                 if false: str contains the Kirchhoff stress or
!                           Lagrange strain
!
!     OUTPUT:
!
!     str(6):     Piola-Kirchhoff stress of the second kind (PK2) or
!                 Euler strain
!
```

The second routine, "stiff2mat.f" converts the tangent stiffness matrix from spatial coordinates into material coordinates.

```
      subroutine stiff2mat(elas,ckl,vj,cauchy)
!
!     converts an element stiffness matrix in spatial coordinates into
!     an element stiffness matrix in material coordinates.
```

```
!
!     INPUT:
!
!     elas(21):   stiffness constants in the spatial description, i.e.
!                 the derivative of the Cauchy stress or the Kirchhoff
!                 stress with respect to the Eulerian strain
!     ckl(3,3):   inverse deformation gradient
!     vj:         Jacobian determinant
!     cauchy:     logical variable
!                 if true: elas is written in terms of Cauchy stress
!                 if false: elas is written in terms of Kirchhoff stress
!
!     OUTPUT:
!
!     elas(21):   stiffness constants in the material description,i.e.
!                 the derivative of the second Piola-Kirchhoff stress (PK2)
!                 with respect to the Lagrangian strain
!
```

8.5.1 ABAQUS umat routines

There are two interfaces to include ABAQUS umat routines: umat_abaqus is meant to include linear materials, umat_abaqusnl for nonlinear materials. For nonlinear materials the logarithmic strain and infinitesimal rotation are calculated, which slows down the calculation. Consequently, the nonlinear routine should only be used if necessary.

The linear routine is triggered by putting ABAQUS in front of the material name. The total length of the material name should not exceed 80 characters, consequently, 74 characters are left for the proper material name. For instance, if the material name in the ABAQUS routine is supposed to be "WOOD", you must specify "ABAQUSWOOD" in the CalculiX input file. The part "ABAQUS" is removed from the name before entering the umat routine.

The nonlinear routine is triggered by putting ABAQUSNL in front of the material name.

Notice that the following fields are not supported so far: sse, spd, scd, rpl, ddsddt, drplde, drpldt, predef, dpred, drot, pnewdt, celent, layer, kspt. If you need these fields, contact "dhondt@t-online.de". Furthermore, the following fields have a different meaning:

- in the linear version:
  - stran:
    - in CalculiX: Lagrangian strain tensor
    - in ABAQUS: logarithmic strain tensor
  - dstran:

    - ∗ in CalculiX: Lagrangian strain increment tensor
    - ∗ in ABAQUS: logarithmic strain increment tensor
  - temp:
    - ∗ in CalculiX: temperature at the end of the increment
    - ∗ in ABAQUS: temperature at the start of the increment
  - dtemp:
    - ∗ in CalculiX: zero
    - ∗ in ABAQUS: temperature increment

- in the nonlinear version:
  - temp:
    - ∗ in CalculiX: temperature at the end of the increment
    - ∗ in ABAQUS: temperature at the start of the increment
  - dtemp:
    - ∗ in CalculiX: zero
    - ∗ in ABAQUS: temperature increment

8.6 User-defined thermal material laws.

Thermal behavior not available in CalculiX can be coded by the user in subroutine "umatht.f". This also applies to any behavior of the thermally equivalent models such as shallow water theory etc. For instance, the thickness of the oil film in lubrication is part of the equivalent conductivity coefficients. A mechanical part can be coupled with the oil region by incorporating the effect of the motion of the mechanical part on the oil film thickness in a thermal material user-subroutine. The header and input/output variables of the umatht routine are as follows:

```
      subroutine umatht(u,dudt,dudg,flux,dfdt,dfdg,
     &  statev,temp,dtemp,dtemdx,time,dtime,predef,dpred,
     &  cmname,ntgrd,nstatv,props,nprops,coords,pnewdt,
     &  noel,npt,layer,kspt,kstep,kinc,vold,co,lakonl,konl,
     &  ipompc,nodempc,coefmpc,nmpc,ikmpc,ilmpc,mi)
!
!     heat transfer material subroutine
!
!     INPUT:
!
!     statev(nstatv)      internal state variables at the start
!                         of the increment
!     temp                temperature at the start of the increment
!     dtemp               increment of temperature
!     dtemdx(ntgrd)       current values of the spatial gradients of the
```

```
!                        temperature
!     time(1)            step time at the beginning of the increment
!     time(2)            total time at the beginning of the increment
!     dtime              time increment
!     predef             not used
!     dpred              not used
!     cmname             material name
!     ntgrd              number of spatial gradients of temperature
!     nstatv             number of internal state variables as defined
!                        on the *DEPVAR card
!     props(nprops)      user defined constants defined by the keyword
!                        card *USER MATERIAL,TYPE=THERMAL
!     nprops             number of user defined constants, as specified
!                        on the *USER MATERIAL,TYPE=THERMAL card
!     coords             global coordinates of the integration point
!     pnewd              not used
!     noel               element number
!     npt                integration point number
!     layer              not used
!     kspt               not used
!     kstep              not used
!     kinc               not used
!     vold(0..4,1..nk)   solution field in all nodes
!                        0: temperature
!                        1: displacement in global x-direction
!                        2: displacement in global y-direction
!                        3: displacement in global z-direction
!                        4: static pressure
!     co(3,1..nk)        coordinates of all nodes
!                        1: coordinate in global x-direction
!                        2: coordinate in global y-direction
!                        3: coordinate in global z-direction
!     lakonl             element label
!     konl(1..20)        nodes belonging to the element
!     ipompc(1..nmpc))   ipompc(i) points to the first term of
!                        MPC i in field nodempc
!     nodempc(1,*)       node number of a MPC term
!     nodempc(2,*)       coordinate direction of a MPC term
!     nodempc(3,*)       if not 0: points towards the next term
!                                  of the MPC in field nodempc
!                        if 0: MPC definition is finished
!     coefmpc(*)         coefficient of a MPC term
!     nmpc               number of MPC's
!     ikmpc(1..nmpc)     ordered global degrees of freedom of the MPC's
!                        the global degree of freedom is
!                        8*(node-1)+direction of the dependent term of
```

```
!                       the MPC (direction = 0: temperature;
!                       1-3: displacements; 4: static pressure;
!                       5-7: rotations)
!     ilmpc(1..nmpc)    ilmpc(i) is the MPC number corresponding
!                       to the reference number in ikmpc(i)
!     mi(1)             max # of integration points per element (max
!                       over all elements)
!     mi(2)             max degree of freedomm per node (max over all
!                       nodes) in fields like v(0:mi(2))...
!
!     OUTPUT:
!
!     u                  not used
!     dudt               not used
!     dudg(ntgrd)        not used
!     flux(ntgrd)        heat flux at the end of the increment
!     dfdt(ntgrd)        not used
!     dfdg(ntgrd,ntgrd)  variation of the heat flux with respect to the
!                        spatial temperature gradient
!     statev(nstatv)     internal state variables at the end of the
!                        increment
!
```

8.7 User-defined nonlinear equations

This user subroutine allows the user to insert his/her own nonlinear equations (also called Multiple Point Constraints or MPC's). The driver routine is "nonlinmpc.f". For each new type of equation the user can define a name, e.g. FUN (maximum length 80 characters). To be consistent, the user subroutine should be called umpc_fun and stored in "umpc_fun.f". In file "nonlinmpc.f" the lines

```
            elseif(labmpc(ii)(1:4).eq.'USER') then
               call umpc_user(aux,aux(3*maxlenmpc+1),const,
     &            aux(6*maxlenmpc+1),iaux,n,fmpc(ii),iit,idiscon)
```

should be duplicated and user (USER) replaced by fun (FUN).

It is assumed that the nonlinear equation is a function of the displacements only. Then it can generally be written as

$$f(u_1, u_2, u_3, ..., u_n) = 0 \tag{358}$$

where u_i represents the displacement in node n_i in direction l_i. Nonlinear equations are solved by approximating them linearly and using an iterative procedure. It is the linearization which must be provided by the user in the

subroutine. Assume we arrived at an intermediate solution $u_1^0, u_2^0, ...u_n^0$. Then the above equation can be linearly approximated by:

$$f(u_1^0, u_2^0, ..., u_n^0) + \sum_{i=1}^{i=n} \left.\frac{\partial f}{\partial u_i}\right|_0 (u_i - u_i^0) = 0 \tag{359}$$

For more details the user is referred to [18]. To use a user-defined equation its name must be specified on the line beneath the keyword *MPC, followed by a list of all the nodes involved in the MPC. This list of nodes is transferred to the user routine, as specified by the following header and input/output variables of the umpc_user routine:

```
      subroutine umpc_user(x,u,f,a,jdof,n,force,iit,idiscon)
!
!     updates the coefficients in a user mpc
!
!     INPUT:
!
!     x(3,n)            Carthesian coordinates of the nodes in the
!                       user mpc.
!     u(3,n)            Actual displacements of the nodes in the
!                       user mpc.
!     jdof              Actual degrees of freedom of the mpc terms
!     n                 number of terms in the user mpc
!     force             Actual value of the mpc force
!     iit               iteration number
!
!     OUTPUT:
!
!     f                 Actual value of the mpc. If the mpc is
!                       exactly satisfied, this value is zero
!     a(n)              coefficients of the linearized mpc
!     jdof              Corrected degrees of freedom of the mpc terms
!     idiscon           0: no discontinuity
!                       1: discontinuity
!                       If a discontinuity arises the previous
!                       results are not extrapolated at the start of
!                       a new increment
!
```

The subroutine returns the value of f ($f(u_1^0, u_2^0, ..., u_n^0)$), the coefficients of the linearization ($\left.\frac{df}{du_i}\right|_0$) and the degrees of freedom involved.

The parameter idiscon can be used to specify whether a discontinuity took place. This usually means that the degrees of freedom in the MPC changed

from the previous call. An example of this is a gap MPC. If a discontinuity occurred in an increment, the results (displacements..) in this increment are NOT extrapolated to serve as an initial guess in the next increment.

An example is given next.

8.7.1 Mean rotation MPC.

This MPC is used to apply a rotation to a set of nodes. The rotation is characterized by its size (angle in radians) and its axis (normal vector). All nodes participating in the rotation should be listed three times (once for each DOF). The user must define an extra node at the end in order to define the size and axis of rotation: the coordinates of the extra node are the components of a vector on the rotation axis, the first DOF of the node is interpreted as the size of the rotation. This size can be defined using a *BOUNDARY card. Applying a mean rotation implies that the mean of the rotation of all participating nodes amounts to a given value, but not the individual rotations per se. The complement of the mean rotation is the torque needed for the rotation. By selecting RF on a *NODE PRINT or *NODE FILE card this torque can be saved in the .dat or .frd file. Conversely, instead of specifying the mean rotation one can also specify the torque (specify a force with *CLOAD on the first DOF of the extra node) and calculate the resulting mean rotation.

```
Example:

*NODE
162,0.,1.,0.
*MPC
MEANROT,3,3,3,2,2,2,14,14,14,39,39,39,42,42,42,
50,50,50,48,48,48,162
..
*STEP
*STATIC
*BOUNDARY
162,1,1,.9
..
*END STEP
```

specifies a mean rotation MPC. Its size is 0.9 radians = 51.56° and the global y-axis is the rotation axis. The participating nodes are 3,2,14,39,42,50 and 48.

Example files: beammr, beammrco.

The theory behind the mean rotation MPC is explained in [18], Section 3.6, in case that all nodes are lying in a plane orthogonal to the rotation axis. If this is not the case, the derivation in [18] is not correct and has to be extended. Indeed, for the general case $\boldsymbol{p}_i'$ and $\boldsymbol{u}_i'$ in Equation (3.98) of that reference have

to be replaced by their projection on a plane orthogonal to the rotation vector $\boldsymbol{a}$. The projection $\boldsymbol{Py}$ of a vector $\boldsymbol{y}$ is given by:

$$\boldsymbol{Py} = \boldsymbol{y} - (\boldsymbol{y} \cdot \boldsymbol{a})\boldsymbol{a}. \tag{360}$$

Defining $\boldsymbol{b}_i \equiv \boldsymbol{Pp}_i'$ Equation (3.101)of the reference has to be replaced by (no implicit summation in this section)

$$\lambda_i = \frac{(\boldsymbol{b}_i \times \boldsymbol{Pu}_i') \cdot \boldsymbol{a}}{\|\boldsymbol{b}_i\| \cdot \|\boldsymbol{b}_i + \boldsymbol{Pu}_i'\|} \tag{361}$$

(recall that the vector product of a vector with itself vanishes). λ_i is the sinus of the angle between $\boldsymbol{Pp}_i'$, which is the projected vector from the center of gravity of the nodal set for which the mean rotation MPC applies to one of its nodes i, and $\boldsymbol{Pp}_i' + \boldsymbol{Pu}_i'$, which is the projection of the vector connecting the deformed position of the center of gravity with the deformed position of node i. The mean rotation in the mean rotation MPC is supposed to be equal to a given angle γ, i.e. the equation to be satisfied is:

$$\sum_{i=1}^{N} \sin^{-1} \lambda_i \equiv \sum_{i=1}^{N} \gamma_i = N\gamma. \tag{362}$$

In order to find the coefficients of the linearization we concentrate here on the derivation of $\frac{\partial \lambda_i}{\partial \boldsymbol{u}_p}$. One readily finds the following relationships:

$$\frac{\partial \|\boldsymbol{y}\|}{\partial \boldsymbol{u}} = \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|} \cdot \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{u}}, \tag{363}$$

$$\frac{\partial \boldsymbol{Py}}{\partial \boldsymbol{u}} = [\boldsymbol{I} - \boldsymbol{a} \otimes \boldsymbol{a}] \cdot \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{u}} \equiv \mathbb{P} \cdot \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{u}}, \tag{364}$$

$$\boldsymbol{a} \cdot (\boldsymbol{y} \times \mathbb{P}) = \boldsymbol{a} \times \boldsymbol{y}. \tag{365}$$

Furthermore, since $\boldsymbol{b}_i + \boldsymbol{Pu}_i' \perp \boldsymbol{a}$ one obtains

$$(\boldsymbol{b}_i + \boldsymbol{Pu}_i') \cdot \mathbb{P} = \boldsymbol{b}_i + \boldsymbol{Pu}_i'. \tag{366}$$

Finally, since (Equation (3.96) of the reference)

$$\boldsymbol{u}_i' = \boldsymbol{u}_i - \frac{1}{N} \sum_j \boldsymbol{u}_j, \tag{367}$$

one further finds

$$\frac{\partial \boldsymbol{u}_i'}{\partial \boldsymbol{u}_p} = \boldsymbol{I} \cdot (\delta_{ip} - \frac{1}{N}), \tag{368}$$

where $\boldsymbol{I}$ is the unit second order tensor. Using the above formulas one arrives at

$$\frac{\partial \lambda_i}{\partial \boldsymbol{u}_p} = \frac{(\delta_{ip} - \frac{1}{N})}{\|\boldsymbol{b}_i + \boldsymbol{P}\boldsymbol{u}'_i\|} \left[\boldsymbol{a} \times \frac{\boldsymbol{b}_i}{\|\boldsymbol{b}_i\|} - \lambda_i \frac{\boldsymbol{b}_i + \boldsymbol{P}\boldsymbol{u}'_i}{\|\boldsymbol{b}_i + \boldsymbol{P}\boldsymbol{u}'_i\|} \right], \tag{369}$$

and

$$\frac{\partial \gamma_i}{\partial \boldsymbol{u}_p} = \frac{1}{\sqrt{1-\lambda_i^2}} \frac{(\delta_{ip} - \frac{1}{N})}{\|\boldsymbol{b}_i + \boldsymbol{P}\boldsymbol{u}'_i\|} \left[\boldsymbol{a} \times \frac{\boldsymbol{b}_i}{\|\boldsymbol{b}_i\|} - \lambda_i \frac{\boldsymbol{b}_i + \boldsymbol{P}\boldsymbol{u}'_i}{\|\boldsymbol{b}_i + \boldsymbol{P}\boldsymbol{u}'_i\|} \right], \tag{370}$$

which replaces Equation (3.109) of the reference.

8.7.2 Maximum distance MPC.

This MPC is used to specify that the (Euclidean) distance between two nodes a and b must not exceed a given distance d. A fictitious node c must be defined using the *NODE card. The distance d should be assigned to the first coordinate of c, the other coordinates are arbitrary. The first DOF of c should be assigned a value of zero by means of a *BOUNDARY card. Since all DOFs of nodes a and b are used in the MPC, these nodes must be listed three times. Notice that due to this MPC discontinuities can arise.

```
Example:

*NODE
262,7.200000,0.,0.
*MPC
DIST,129,129,129,10,10,10,262
..
*STEP
*STATIC
*BOUNDARY
262,1,1,0.
..
*END STEP
```

specifies a maximum distance MPC. The distance between nodes 129 and 10 is not allowed to exceed 7.2 units.

Example file: dist.

8.7.3 Gap MPC.

Internally, a gap element is handled by a gap MPC. However, the user access is realized by the *ELEMENT and *GAP cards and not by a *MPC card.

9 Program structure.

First an important remark: starting with version 2.8 the environment variable CCX_LOG_ALLOC has been introduced. If set to 1 (default is zero) one gets detailed information on all allocated, reallocated and deallocated fields during the executation of CalculiX. This may be particularly important during debugging of segmentation faults.

CalculiX CrunchiX is a mixture of FORTRAN77 (with elements from FORTRAN90) and C. C is primarily used for automatic allocation and reallocation purposes. FORTRAN is the first language I learned and I must admit that I'm still a FORTRAN addict. I use C where necessary, I avoid it where possible. Another option would have been to code everything in FORTRAN90, however, to this date there is no good FREE FORTRAN90 compiler. Roughly speaking, the main routine and some of the routines called by main are in C, the others are in FORTRAN. This means that no C routine is called by a FORTRAN routine, a FORTRAN routine may be called by a C routine or a FORTRAN routine. There are NO commons in the code. All data transfer is through arguments of subroutine calls. All arguments are transferred by address, not value (there may be one or two exceptions on this rule in the code).

The main subroutine of CalculiX is ccx_2.8p2.c. It consists roughly of the following parts:

- Allocation of the fields

For each step:

1. Reading the step input data (including the prestep data for the first step)
2. Determining the matrix structure
3. Filling and solving the set of equations, storing the results.

9.1 Allocation of the fields

This section consists of three subroutine calls:

- openfile
- readinput
- allocation

9.1.1 openfile

In this subroutine the input (.inp) and output files (.dat, .frd, .sta, .cvg) are opened. The .dat file contains data stored with *NODE PRINT and *EL PRINT, the .frd file contains data stored with *NODE FILE and *EL FILE, the .sta and .cvg file contain information on the convergence of the calculation.

9.1.2 readinput

This subroutine reads the input and stores it in field inpc. Before storing, the following actions are performed:

- the blanks are deleted
- all characters are changed to uppercase except file names
- the comment lines are not stored
- the include statements are expanded

Furthermore, the number of sets are counted and stored in nset_, the number of lines in inpc are stored in nline. The variable nset_ is used for subsequent allocation purposes. Finally, the order in which inpc is to be read is stored in the fields ipoinp and inp. Indeed, some keyword cards cannot be interpreted before others were read, e.g. a material reference in a *SOLID SECTION card cannot be interpreted before the material definition in the *MATERIAl card was read. The order in which keyword cards must be read is defined in field nameref in subroutine keystart.f. Right now, it reads:

1. *RESTART,READ
2. *NODE
3. *ELEMENT
4. *NSET
5. *ELSET
6. *TRANSFORM
7. *MATERIAL
8. *ORIENTATION
9. *SURFACE
10. *TIE
11. *SURFACE INTERACTION
12. *INITIAL CONDITIONS
13. *AMPLITUDE
14. *CONTACTPAIR
15. everything else

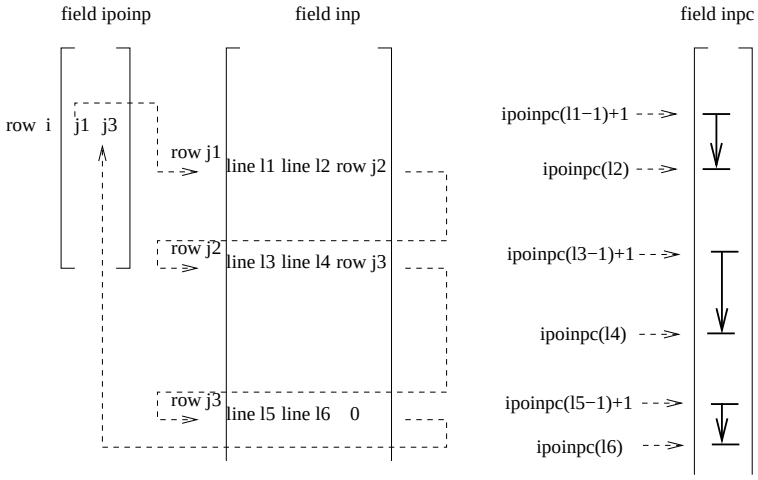


Figure 134: Reading the lines for keyword entry i

This means that *RESTART,READ has to be read before all other cards, then comes *NODE etc. The way inpc is to be read is stored in the fields ipoinp, inp and ipoinpc. The two-dimensional field ipoinp consists of 2 columns and nentries rows, where nentries is the number of keyword cards listed in the list above, i.e. right now nentries=15. The first column of row i in field ipoinp contains a row number of field inp, for instance j1. Then, the first column of row j1 in field inp contains the line number where reading for keyword i should start, the second column contains the line number where reading should end and the third column contains the line number in field inp where the reading information for keyword i continues, else it is zero. If it is zero the corresponding row number in inp is stored in the second column of row i in field ipoinp. Lines are stored consecutively in field inpc (without blanks and without comment lines). Line l1 starts at ipoinpc(l1-1)+1 (first character) and ends at ipoinpc(l1) (last character). Notice that ipoinpc(0)=0. This structure uniquely specifies in what order field inpc must be read. This is also illustrated in Figure 134

If you want to add keywords in the above list you have to

- update nentries in the parameter statement in the FORTRAN subroutines allocation.f, calinput.f, keystart.f, getnewline.f and writeinput.f
- update the initialization of nentries in the C-routines ccx_2.8p2.c and readinput.c.
- update the data statement for the field nameref in the FORTRAN subroutines keystart.f and writeinput.f
- update the data statement for the field namelen in the FORTRAN subroutine keystart.f. It contains the number of characters in each keyword.

- look for the block running

```
      else if(strcmp1(&buff[0],"*AMPLITUDE")==0){
        FORTRAN(keystart,(&ifreeinp,ipoinp,inp,"AMPLITUDE",
                          nline,&ikey));
}
```

  in file readinput.c, copy the block and replace AMPLITUDE by the new keyword.

9.1.3 allocate

In the subroutine allocate.f the input is read to determine upper bounds for the fields in the program. These upper bounds are printed so that the user can verify them. These upper bounds are used in the subsequent allocation statements in ccx_2.8p2.c. This procedure might seem slightly awkward, however, since the subroutines reading the input later on are in FORTRAN77, a reallocation is not possible at that stage. Therefore, upper bounds must have been defined.

It is important to know where fields are allocated, reallocated and deallocated. Most (re-, de-) allocation is done in ccx_2.8p2.c. Table (19) gives an overview where the allocation (A), reallocation (R) and deallocation (D) is done in file ccx_2.8p2.c. A fundamental mark in this file is the call of subroutine calinput, where the input data is interpreted. A couple of examples: field kon contains the topology of the elements and is allocated with size nkon, which is an upper bound estimate, before all steps. After reading the input up to and including the first step in subroutine calinput the field is reallocated with the correct size, since at that point all elements are read and the exact size is known. This size cannot change in subsequent steps since it is not allowed to define new elements within steps. The field xforc is allocated with the upper bound estimate nforc_ before entering subroutine calinput. After reading the input up to and including the first step its size is reallocated with the true size nforc. Before entering calinput to read the second step (or any subsequent step) xforc is reallocated with size nforc_, since new forces can be defined in step two (and in any subsequent step). After reading step two, the field is reallocated with the momentary value of nforc, and so on. All field which can change due to step information must be reallocated in each step.

Table 19: Allocation table for file ccx_2.8p2.c.

	before calinput		after calinput				size
	$<$ step 1	$>$ step 1	= step 1	$>$ step 1	$\geq$ step 1	step 1 or ntrans $>$ 0	
co	A	R			R		3*nk
kon	A		R				nkon
ipkon	A		R				ne
lakon	A		R				8*ne
ielprop	A		nprop>0: R else D		nprop $>$ 0 and network = 1: R		ne
prop	A		nprop>0: R else D				nprop
nodeboun	A	R			R		nboun
ndirboun	A	R			R		nboun
typeboun	A	R			R		nboun
xboun	A	R			R		nboun
ikboun	A	R			R		nboun
ilboun	A	R			R		nboun
iamboun	A	nam $>$ 0: R	nam $\leq$ 0: D		nam $>$ 0: R		nboun
nodebounold	irstrt $<$ 0: A		A	R/R			nboun
ndirbounold	irstrt $<$ 0: A		A	R/R			nboun
xbounold	irstrt $<$ 0: A		A	R/R			nboun
ipompc	A	R			R		nmpc
labmpc	A	R			R		20*nmpc+1
ikmpc	A	R			R		nmpc
ilmpc	A	R			R		nmpc
fmpc	A	R			R		nmpc
nodempc	A						3*memmpc_
coefmpc	A						memmpc_

Table 19: (continued)

	before calinput		after calinput				size
	$<$ step 1	$>$ step 1	= step 1	$>$ step 1	$\geq$ step 1	step 1 or ntrans > 0	
nodeforc	A	R			R		2*nforc
ndirforc	A	R			R		nforc
xforc	A	R			R		nforc
ikforc	A	R			R		nforc
ilforc	A	R			R		nforc
iamforc	A	nam $>$ 0: R	nam $\leq$ 0: D		nam $>$ 0: R		nforc
xforcold		irstr $<$ 0: A	A	R			nforc
idefforc	A	A			D		
nelemload	A	R			network =1: R		2*nload
sideload	A	R			network =1:R		20*nload
xload	A	R			network =1:R		2*nload
iamload	A	nam $>$ 0: R	nam $\leq$ 0: D		nam $>$ 0 network = 1: R		2*nload
xloadold		irstrt $<$ 0: A	A	R	network =1: R		2*nload
idefload	A	A			D		
cbody	A	R			R		81*nbody
ibody	A	R			R		3*nbody
xbody	A	R			R		7*nbody
xbodyold	A	R			R		7*nbody
idefbody	A	A			D		
nodeflow	A	R			R		2*nflow
xflow	A	R			R		nflow
iamflow	A	nam $>$ 0: R	nam $\leq$ 0: D		nam $>$ 0: R		nflow
xflowold			A	R			2*nflow
nodeprint	A	R			R		noprint
nelemprint	A	R			R		neprint

Table 19: (continued)

	before calinput		after calinput				size
	$<$ step 1	$>$ step 1	= step 1	$>$ step 1	$\geq$ step 1	step 1 or ntrans $>$ 0	
noelplab	A						4*nlabel
noelflab	A						4*nlabel
filab	A						
prlab	A						
prset	A						
set	A		R				81*nset
istartset	A		R				nset
iendset	A		R				nset
ialset	A		R				nalset
elcon	A		R				(ncmat_+1)* *ntmat_*nmat
nelcon	A		R				2*nmat
rhcon	A		R				2*ntmat_*nmat
nrhcon	A		R				nmat
shcon	A		R				4*ntmat_*nmat
nshcon	A		R				nmat
cocon	A		R				7*ntmat_*nmat
ncocon	A		R				nmat

Table 19: (continued)

	before calinput		after calinput				size
	$<$ step 1	$>$ step 1	= step 1	$>$ step 1	$\geq$ step 1	step 1 or ntrans $>$ 0	
alcon	A		R				7*ntmat_*nmat
nalcon	A		R				2*nmat
alzero	A		R				nmat
plicon	A		npmat_ $>$ 0: R else: D				(2*npmat_+1)* *ntmat_*nmat
nplicon	A		npmat_ $>$ 0: R else: D				(ntmat_+1)*nmat
plkcon	A		npmat_ $>$ 0: R else: D				(2*npmat_+1)* *ntmat_*nmat
nplkcon	A		npmat_ $>$ 0: R else: D				(ntmat_+1)*nmat
orname	A		norien $>$ 0: R else:D				80*norien
orab	A		norien $>$ 0: R else:D				7*norien
ielorien	A		norien $>$ 0: R else:D		norien $>$ 0 and network = 1: R		mi[2]*ne
trab	A		ntrans $>$ 0: R else:D				7*ntrans
inotr	A	ntrans $>$ 0: R	ntrans $\leq$ 0: D		ntrans $>$ 0: R		2*nk
amname	A	nam $>$ 0: R	nam $>$ 0: R else:D	nam $>$ 0: R			80*nam
amta	A	nam $>$ 0: R	nam $>$ 0: R else:D	nam $>$ 0: R			2*namta* (3*nam-2)
namta	A	nam $>$ 0: R	nam $>$ 0: R else:D	nam $>$ 0: R			3*nam

Table 19: (continued)

	before calinput		after calinput				size
	$<$ step 1	$>$ step 1	= step 1	$>$ step 1	$\geq$ step 1	step 1 or ntrans $>$ 0	
t0	A	ithermal $\neq$ 0 R	ithermal = 0: D		ithermal $\neq$ 0 R		nk (3D) 3*nk_ (1D/2D)
t1	A	ithermal $\neq$ 0 R	ithermal = 0: D		ithermal $\neq$ 0 R		nk (3D) 3*nk_ (1D/2D)
iamt1	A	ithermal $\neq$ 0: R	nam $\leq$ 0 or ithermal = 0: D		ithermal $\neq$ 0 and nam $>$ 0: R		nk
t1old		irstrt $<$ 0, ithermal $\neq$ 0: A	ithermal $\neq$ 0: A	ithermal $\neq$ 0: R			nk
t0g	if 1D/2D: A	if 1D/2D and ithermal $\neq$ 0: R	if 1D/2D and ithermal = 0: D		if 1D/2D ithermal $\neq$ 0: R		2*nk
t1g	if 1D/2D: A	if 1D/2D and ithermal $\neq$ 0: R	if 1D/2D and ithermal = 0: D		if 1D/2D ithermal $\neq$ 0: R		2*nk
ielmat	A		R				mi[2]*ne
matname	A		R				80*nmat
vold	A	R	R	R			mt*nk
veold	A	nmethod $\neq$ 4 and (nmethod $\neq$ 1 or iperturb $<$ 2): A else: R			nmethod = 4/5 or ($\|$nmethod$\|$ = 1 and iperturb $\geq$ 2): R else: D		mt*nk
accold					nmethod = 4 and iperturb $>$ 1: A		4*nk
only if ne1d $\neq$ 0 or ne2d $\neq$ 0							
iponor	A		R				2*nkon
xnor	A		R				infree[0]
knor	A		R				infree[1]
thickn	A		D				-
thicke	A		R				mi[2]*nkon
offset	A		R		network=1: R		2*ne
iponoel	A		R				infree[3]
inoel	A		R				3*(infree[2]-1)
rig	A		R				infree[3]

Table 19: (continued)

	before calinput		after calinput				size
	$<$ step 1	$>$ step 1	= step 1	$>$ step 1	$\geq$ step 1	step 1 or ntrans $>$ 0	
ics	ncs_ $>$ 0 or		R				ncs_
	npt_ $>$ 0: A		R				
dcs	ncs_ $>$ 0 or		D				-
	npt_ $>$ 0: A		D				
cs	ntie_ $>$ 0: A		mcs $>$ 0: R else: D				
sti		irstrt $<$ 0: A	A		network = 1: R		6*mint_*ne
eme		irstrt $<$ 0: A	A		network = 1: R		6*mint_*ne
ener		irstrt $<$ 0 and nener=1: A			nener=1 and nenerold=0: A		mint_*ne*2
xstate	A		R				nstate_ * *mint_ * ne_
tieset	ntie $\geq$ 0: A						
tietol	ntie $\geq$ 0: A						
prestr	A		iprestr = 1/2: R else:D		iprestr $>$ 0 and		6*mi[0]*ne

Note: ithermal(1) and ithermal are in this manual synonymous.

9.2 Reading the step input data

For each step the input data are read in subroutine calinput.f. For the first step this also includes the prestep data. The order in which the data is read was explained in the previous section (fields ipoinp and inp).

For each keyword card there is a subroutine, most of them are just the keyword with the letter 's' appended. For instance, *STEP is read in subroutine steps.f, *MATERIAL in materials.f. Some obey the plural building in English: *FREQUENCY is read in frequencies.f. Some are abbreviated: *CYCLIC SYMMETRY MODEL is read in cycsymmods.f. Treating more than 60 keyword cards accounts in this way for roughly one fourth of all subroutines.

At this point it may be useful to talk about a couple of important structures in the code.

9.2.1 SPC's

The first one is the cataloguing algorithm for SPC's (single point constraints, *BOUNDARY). Let's say a boundary condition m is defined for node i in direction j, $0 \leq j \leq 6$, direction 0 stands for temperature, directions 1 to 3 for translations in global x-, y- and z- direction, direction 4 stands for static pressure, directions 5 to 7 stand for rotations about the global x-, y- and z-axis. Then a degree of freedom idof $= 8 * (i-1) + j$ is assigned to this boundary condition. Then, it is stored at location k in the one-dimensional field ikboun, where all previous boundary degrees of freedom are stored in numerical order such that ikboun$(k-1) <$ idof $<$ ikboun$(k+1)$. Furthermore the number of the boundary condition (m) is stored in ilboun: ilboun(k)=m, and the node of the boundary condition, its direction and value are stored in the one-dimensional fields nodeboun, ndirboun and xboun: nodeboun$(m) = i$, ndirboun$(m) = j$ and xboun(m) = value. If an amplitude definition applies to the boundary condition, its number n is stored in the one-dimensional field iamboun: iamboun$(m) = n$.

The SPC type is stored in the one-dimensional field typeboun. SPC's can be of different types, depending on whether the were defined by a genuin *BOUNDARY CARD, or introduced for other reasons. The field typeboun is a one-dimensional character*1 field. Other reasons to introduce SPC's are:

- fixing of the midplane in expanded plane stress/plane strain/axisymmetric elements
- taking care of the inhomogeneous term in nonlinear MPC's such as the PLANE *MPC, the STRAIGHT *MPC, a *RIGID BODY definition or USER *MPC.

The corresponding type code is:

- B = prescribed boundary condition
- M = midplane constraint (plane stress/plane strain/axisymmetric elements)

- P = PLANE MPC
- R = RIGID BODY definition
- S = STRAIGHT MPC
- U = USER MPC

The total number of boundary conditions is stored in variable nboun.

Consequently, ikboun contains all degrees of freedom of the boundary conditions in numerical order, and ilboun contains the corresponding boundary condition numbers. This assures that one can quickly check whether a given degree of freedom was used in a SPC. For example, if the SPC's look like:

```
*BOUNDARY
8,1,1,0.
10,1,2,0.
7,3,3,-1.
```

the fields look like:

$$\text{nodeboun} = \begin{Bmatrix} 8 \\ 10 \\ 10 \\ 7 \end{Bmatrix}, \text{ndirboun} = \begin{Bmatrix} 1 \\ 1 \\ 2 \\ 3 \end{Bmatrix}, \text{xboun} = \begin{Bmatrix} 0. \\ 0. \\ 0. \\ -1. \end{Bmatrix} \tag{371}$$

$$\text{typeboun} = \begin{Bmatrix} B \\ B \\ B \\ B \end{Bmatrix}, \text{ikboun} = \begin{Bmatrix} 45 \\ 50 \\ 64 \\ 65 \end{Bmatrix}, \text{ilboun} = \begin{Bmatrix} 4 \\ 1 \\ 2 \\ 3 \end{Bmatrix}. \tag{372}$$

and nboun=4.

Finally, the following one-dimensional fields are also used:

- nodebounold: contains the node numbers of the SPC's at the end of the last step
- ndirbounold: contains the directions of the SPC's at the end of the last step
- xbounold: contains the values of the SPC's at the end of the last step, or, if this is the first step, zero values.
- xbounact: contains the values of the SPC's at the end of the present increment, or, for linear calculations, at the end of the present step. The field xbounact is derived from the fields xbounold and xboun by use of the present time and/or amplitude information. How this is done depends on the procedure and is explained later on.

- xbounini: contains the values of the SPC's at the end of the last increment, or, if this is the first increment in the first step, zero's. This field is used for nonlinear calculations only.

Notice that among the boundary conditions SPC's are somewhat special. They are sometimes called geometric boundary conditions to distinguish them from the natural boundary conditions such as the application of a concentrated or distributed load. To remove a natural boundary condition, just set it to zero. This is not true for geometric boundary conditions: by setting a SPC to zero, the corresponding node is fixed in space which usually does not correspond to what one understands by removing the SPC, i.e. free unconstrained motion of the node. Therefore, to remove a SPC the option OP=NEW must be specified on the *BOUNDARY keyword card. This removes ALL SPC constraints. Then, the constraints which the user does not wish to remove must be redefined. Depending on the procedure (*STATIC, *DYNAMIC...), the change of SPC's is applied in a linear way. This means that the old SPC information must be kept to establish this linear change. That's why the fields nodebounold and ndirbounold are introduced. The relationship between the old and new SPC's is established in subroutine spcmatch, called from ccx_2.8p2.c.

9.2.2 Homogeneous linear equations

Homogeneous linear equations are of the form

$$a_1 u_{i_1} + a_2 u_{i_2} + \ldots + a_n u_{i_n} = 0. \tag{373}$$

The variable n can be an arbitrary integer, i.e. the linear equation can contain arbitrarily many terms. To store these equations (also called MPC's) the one-dimensional field ipompc and the two-dimensional field nodempc, which contains three columns, are used. For MPC i, row i in field ipompc contains the row in field nodempc where the definition of MPC i starts: if $ipompc(i) = j$ then the degree of freedom of the first term of the MPC corresponds to direction $nodempc(j, 2)$ in node $nodempc(j, 1)$. The coefficient of this term is stored in $coefmpc(j)$. The value of $nodempc(j, 3)$ is the row in field nodempc with the information of the next term in the MPC. This continues until $nodempc(k, 3) = 0$ which means that the term in row k of field nodempc is the last term of MPC i.

For example, consider the following MPC:

$$5.u_1(10) + 3.u_1(147) + 4.5u_3(58) = 0. \tag{374}$$

where $u_1(10)$ stands for the displacement in global x-direction of node number 10, similar for the other terms. Assume this MPC is equation number i. Then, the storage of this equation could look like in Figure 135.

The first term in a MPC is special in that it is considered to be the dependent term. In the finite element calculations the degree of freedom corresponding to such a dependent term is written as a function of the other terms and is removed

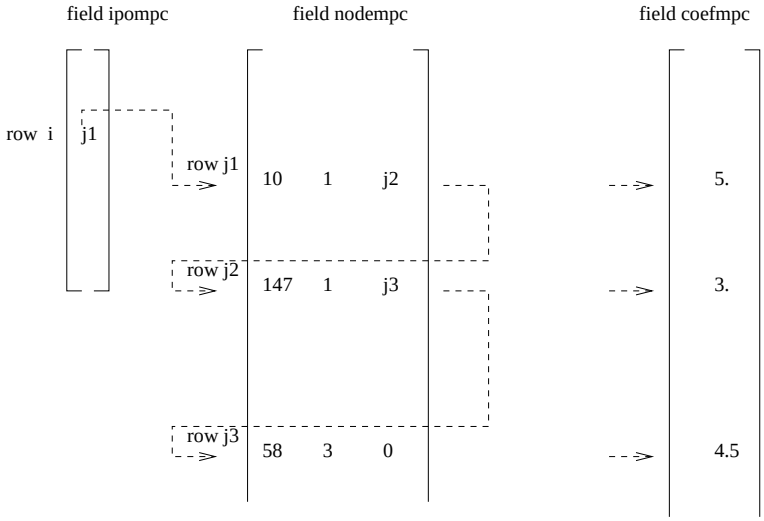


Figure 135: Example of the storage of a linear equation

from the system of equations. Therefore, no other constraint can be applied to the DOF of a dependent term. The DOF's of the dependent terms of MPC's are catalogued in a similar way as those corresponding to SPC's. To this end, a one-dimensional field ikmpc is used containing the dependent degrees of freedom in numerical order, and a one-dimensional field ilmpc containing the corresponding MPC number. The meaning of these fields is completely analogous to ikboun and ilboun and the reader is referred to the previous section for details.

In addition, MPC's are labeled. The label of MPC i is stored in $labmpc(i)$. This is a one-dimensional field consisting of character words of length 20 (in FORTRAN: character*20). The label is used to characterize the kind of MPC. Right now, the following kinds are used:

- CYCLIC: denotes a cyclic symmetry constraint
- MEANROT: denotes a mean rotation constraint
- PLANE: denotes a plane constraint
- RIGID: denotes a rigid body constraint
- STRAIGHT: denotes a straight constraint
- SUBCYCLIC: denotes a linear MPC some terms of which are part of a cyclic symmetry constraint

The MEANROT, PLANE and STRAIGHT MPC's are selected by the *MPC keyword card, a RIGID MPC is triggered by the *RIGID BODY keyword card,

and a CYCLIC MPC by the *CYCLIC SYMMETRY MODEL card. A SUB-CYCLIC MPC is not triggered explicitly by the user, it is determined internally in the program.

Notice that non-homogeneous MPC's can be reduced to homogeneous ones by introducing a new degree of freedom (introduce a new fictitious node) and assigning the inhomogeneous term to it by means of a SPC. Nonlinear MPC's can be transformed in linear MPC's by linearizing them [18]. In CalculiX this is currently done for PLANE MPC's, STRAIGHT MPC's, USER MPC's and RIGID BODY definitions. Notice that SPC's in local coordinates reduce to linear MPC's.

Finally, there is the variable icascade. It is meant to check whether the MPC's changed since the last iteration. This can occur if nonlinear MPC's apply (e.g. a coefficient is at times zero and at other times not zero) or under contact conditions. This is not covered yet. Up to now, icascade is assumed to take the value zero, i.e. the MPC's are not supposed to change from iteration to iteration. (to be continued)

9.2.3 Concentrated loads

Concentrated loads are defined by the keyword card *CLOAD. The internal structure to store concentrated loads is very similar to the one for SPC's, only a lot simpler. The corresponding one-dimensional field for nodeboun, ndirboun, xboun, iamboun, ikboun and ilboun are nodeforc, ndirforc, xforc, iamforc, ikforc and ilforc. The actual number of concentrated loads is nforc, an estimated upper bound (calculated in subroutine allocation.f) is nforc_. The field xforcold and xforcact are the equivalent of xbounold and xbounact, respectively. There is no equivalent to nodebounold, ndirbounold, xbounini and typeboun. These fields are not needed. Indeed, if the option OP=NEW is specified on a *CLOAD card, all values in xboun are set to zero, but the entries in nodeforc and ndirforc remain unchanged. Notice that DOF zero (heat transfer calculations) has the meaning of concentrated heat source.

9.2.4 Facial distributed loads

The field architecture discussed here applies to loads on element faces and heat sources per unit of mass. Consequently, it is used for the following keyword cards:

- *DFLUX: S and BF load labels
- *DLOAD: P load labels
- *FILM: F load labels
- *RADIATE: R load labels
- *TRANSFORMF: T load labels. This label only applies to CFD-calculations, for which transformations are applied to element faces (and not to nodes as for others types of calculations).

It does not apply to gravity and centrifugal loads. These are treated separately.

The two-dimensional integer field nelemload contains two columns and as many rows as there are distributed loads. Its first column contains the element number the load applies to. Its second column is only used for forced convection in which case it contains the fluid node number the element exchanges heat with. The load label is stored in the one-dimensional field sideload (maximum 20 characters per label). The two-dimensional field xload contains two columns and again as many rows as there are distributed loads. For *DFLUX and *DLOAD the first column contains the nominal loading value, the second column is not used. For *FILM and *RADIATE loads the first column contains the nominal film coefficient and the emissivity, respectively, and the second column contains the sink temperature. For forced convection, cavity radiation and non uniform loads some of the above variables are calculated during the program execution and the predefined values in the input deck are not used. The nominal loading values can be changed by defining an amplitude. The number of the amplitude (in the order of the input deck) is stored in the one-dimensional field iamload. Based on the actual time the actual load is calculated from the nominal value and the amplitude, if any. It is stored in the one-dimensional field xloadact.

In the subroutine calinput.f, the distributed loads are ordered according to the element number they apply to. Accordingly, the first load definition in the input deck does not necessarily correspond to the first row in fields nelemload, xload, iamload, xloadact and sideload.

As an example, assume the following distributed loads:

```
*DLOAD
10,P3,8.3
*FILM
6,F4,273.,10.
12,F4FC,20,5.
```

then the loading fields will look like:

$$\text{nelemload} = \begin{bmatrix} 6 & 0 \\ 10 & 0 \\ 12 & 20 \end{bmatrix}, \text{xload} = \begin{bmatrix} 10. & 273. \\ 8.3 & 0. \\ 5. & 0. \end{bmatrix}. \tag{375}$$

$$\text{sideload} = \begin{Bmatrix} F4 \\ P3 \\ F4FC \end{Bmatrix}, \text{iamload} = \begin{Bmatrix} 0 \\ 0 \\ 0 \end{Bmatrix}. \tag{376}$$

9.2.5 Mechanical body loads

The field architecture discussed here applies to centrifugal loads and gravity loads. Consequently, it is used for the *DLOAD card with the following labels:

- CENTRIF: centrifugal load

- GRAV: gravity load with known gravity vector
- NEWTON: generalized gravity

The two-dimensional integer field ibody contains three columns and as many rows as there are body loads. Its first column contains a code identifying the kind of load:

- 1 = centrifugal load
- 2 = gravity load with known gravity vector
- 3 = generalized gravity

Its second column contains the number of the amplitude to be applied, if any. The third column contains the load case. This is only important for steady state dynamics calculations with harmonic loading. The default values is 1 and means that the loading is real (in-phase); if the value is 2 the loading is imaginary (out-of-phase). The element number or element set, for which the load is defined is stored in the one-dimensional character field cbody. It contains as many entries as there are body loads. The nominal value of the body load is stored in the first column of field xbody. This is a two-dimensional field containing 7 columns and as many rows as there are body loads. The second to fourth column is used to store a point on the centrifugal axis for centrifugal loads and the normalized gravity vector for gravity loading. If the gravity vector is not known and has to be determined by the mass distribution in the structure (also called generalized gravity) columns two to seven remain undefined. This also applies to columns five to seven for non-generalized gravity loading. For centrifugal loading columns five to seven of field xbody contain a normalized vector on the centrifugal axis.

Based on the actual time the actual body load is calculated from the nominal value and the amplitude, if any. It is stored in the first column of field xbodyact. Columns two to seven of xbodyact are identical to the corresponding columns of xbody.

The body loads are not stored in the order in which they are defined in the input deck. Rather, they are ordered in alphabetical order according to the element number or element set name they apply to. An element number is interpreted as a character.

As an example, assume the following body loads:

```
*DLOAD
Eall,CENTRIF,1.E8,0.,0.,0.,1.,0.,0.
8,GRAV,9810.,0.,0.,-1.
E1,NEWTON
```

then the loading fields will look like:

$$\text{ibody} = \begin{bmatrix} 2 & 0 & 1 \\ 3 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}, \text{cbody} = \begin{Bmatrix} 8 \\ \text{E1} \\ \text{Eall} \end{Bmatrix}, \tag{377}$$

$$\text{xbody} = \begin{bmatrix} 9810. & 0. & 0. & -1. & 0. & 0. & 0. \\ 0. & 0. & 0. & 0. & 0. & 0. & 0. \\ 1.E8 & 0. & 0. & 0. & 1. & 0. & 0. \end{bmatrix}. \tag{378}$$

9.2.6 Sets

A set is used to group nodes or elements. In the future, it will also be used to define surface based on nodes and surfaces based on element faces. A set i is characterized by its name set(i) and two pointers istartset(i) and iendset(i) pointing to entries in the one-dimensional field ialset. The name set(i) consists of at most 21 characters, the first twenty of which can be defined by the user. The last character is 'N' for a node set and 'E' for an element set. For surfaces, which are internally treated as sets, these characters are 'S' for nodal surfaces and 'T' for element facial surfaces. The extra character allows the user to choose identical names for node and elements sets and/or surfaces. The nodes or elements a set consists of are stored in field ialset between row istartset(i) and row iendset(i). If the parameter GENERATE was not used in the set definition, the entries in ialset are simply the node or element numbers. If GENERATE is used, e.g.

```
*NSET,NSET=N1,GENERATE
20,24
```

the start number, the end number and increment preceded by a minus sign are stored, in that order. Accordingly, for the above example: 20,24,-1. Consequently, a negative number in field ialset always points to an increment to be used between the two preceding entries. For example, if the only two sets are defined by:

```
*NSET,NSET=N1,GENERATE
20,24
*NSET,NSET=N1
383,402,883
*ELSET,ELSET=N1,GENERATE
3,8
```

the fields set, istartset, iendset and ialset read:

$$\text{set} = \begin{Bmatrix} N1N \\ N1E \end{Bmatrix}, \text{istartset} = \begin{Bmatrix} 1 \\ 7 \end{Bmatrix}, \text{iendset} = \begin{Bmatrix} 6 \\ 9 \end{Bmatrix}, \text{ialset} = \begin{Bmatrix} 20 \\ 24 \\ -1 \\ 383 \\ 402 \\ 883 \\ 3 \\ 8 \\ -1 \end{Bmatrix}. \tag{379}$$

9.2.7 Material description

The size of the fields reserved for material description is governed by the scalars nmat_, nmat, ncmat_, ntmat_ and npmat_. Their meaning:

- nmat_: upper estimate of the number of materials
- nmat: actual number of materials
- ncmat_: maximum number of (hyper)elastic constants at any temperature for any material
- ntmat_: maximum number of temperature data points for any material property for any material
- npmat_: maximum number of stress-strain data points for any temperature for any material for any type of hardening (isotropic or kinematic)

An elastic material is described by the two-dimensional integer field nelcon and three-dimensional real field elcon. For material i, nelcon(1,i) contains for linear elastic materials the number of elastic constants. For hyperelastic materials and the elastic regime of viscoplastic materials nelcon(1,i) contains an integer code uniquely identifying the material. The code reads a follows:

- -1: Arruda-Boyce
- -2: Mooney-Rivlin
- -3: Neo-Hooke
- -4: Ogden (N=1)
- -5: Ogden (N=2)
- -6: Ogden (N=3)
- -7: Polynomial (N=1)
- -8: Polynomial (N=2)
- -9: Polynomial (N=3)
- -10: Reduced Polynomial (N=1)
- -11: Reduced Polynomial (N=2)
- -12: Reduced Polynomial (N=3)
- -13: Van der Waals (not implemented yet)
- -14: Yeoh
- -15: Hyperfoam (N=1)

- -16: Hyperfoam (N=2)
- -17: Hyperfoam (N=3)
- -50: deformation plasticity
- -51: incremental plasticity (no viscosity)
- -52: viscoplasticity
- $<$ -100: user material routine with -kode-100 user defined constants with keyword *USER MATERIAL

Notice that elconloc is also used to store

- user-defined constants for user-defined materials
- the creep constants for isotropic viscoplastic materials (after the two elastic constants).

Entry nelcon(2,i) contains the number of temperature points for material i.

The field elcon is used for the storage of the elastic constants: elcon(0,j,i) contains the temperature at the (hyper)elastic temperature point j of material i, elcon(k,j,i) contains the (hyper)elastic constant k at temperature point j of material i. Notice that the first index of field elcon starts at zero.

Suppose only one material is defined:

```
*MATERIAL,NAME=EL
*ELASTIC
210000.,.3,293.
200000.,.29,393.
180000.,.27,493.
```

then the fields nelcon and elcon look like:

$$\text{nelcon} = \begin{bmatrix} 2 & 3 \end{bmatrix}, \text{elcon}(*,*,1) = \begin{bmatrix} 293. & 393. & 493. \\ 210000. & 200000. & 180000 \\ .3 & .29 & .27 \end{bmatrix}, \tag{380}$$

and nmat=1, ntmat_ = 3, ncmat_=2.

Other material properties are stored in a very similar way. The expansion coefficients are stored in fields nalcon and alcon, the conductivity coefficients in fields ncocon and cocon. The density and specific heat are stored in fields nrhcon, rhcon, nshcon and shcon, respectively. Furthermore, the specific gas constant is also stored in shcon. The fields nrhcon and nshcon are only one-dimensional, since there is only one density and one specific heat constant per temperature per material (the specific gas constant is temperature independent).

The isotropic hardening curves for viscoplastic materials are stored in the two-dimensional integer field nplicon and the three-dimensional real field plicon.

The entry nplicon(0,i) contains the number of temperature data points for the isotropic hardening definition of material i, whereas nplicon(j,i) contains the number of stress-strain data points at temperature point j of material i. Entry plicon(2*k-1,j,i) contains the stress corresponding to stress-plastic strain data point k at temperature data point j of material i, plicon(2*k,j,i) contains the plastic strain corresponding to stress-plastic strain data point k at temperature data point j of material i. Similar definitions apply for the kinematic hardening curves stored in nplkcon and plkcon.

9.3 Expansion of the one-dimensional and two-dimensional elements

Typical one-dimensional elements are beams, typical two-dimensional elements are shells, plane stress elements, plane strain elements and axisymmetric elements. Their dimension in thickness direction (for two-dimensional elements) or orthogonal to their axis (for beam elements) is much smaller than in the other directions. In CalculiX these elements are expanded to volume elements. Only quadratic shape functions are accepted.

The expansion of the elements requires several steps:

- cataloguing the elements belonging to one and the same node
- calculating the normals in the nodes
- generating the expanded volume elements
- taking care of the connection of 1D/2D elements with genuine 3D elements
- applying the SPC's to the expanded structure
- applying the MPC's to the expanded structure
- applying the temperatures and temperature gradients
- applying nodal forces to the expanded structure

9.3.1 Cataloguing the elements belonging to a given node

A node can belong to several elements of different types. The structure to store this dependence consists of two fields: a one-dimensional field iponoel and a two-dimensional field inoel. For node i the value j1=iponoel(i) points to row j1 in field inoel containing in its first column the number k1 of an element to which node i belongs, in its second column the local number l1 which node i assumes in the topology of the element and in its third column the row number j2 in field inoel where another element to which node i belongs is listed. If no further element exists, this entry is zero (Figure 136).

Notice that this structure allows the node to belong to totally different element types, e.g. a beam element, a shell element and a plane stress element.

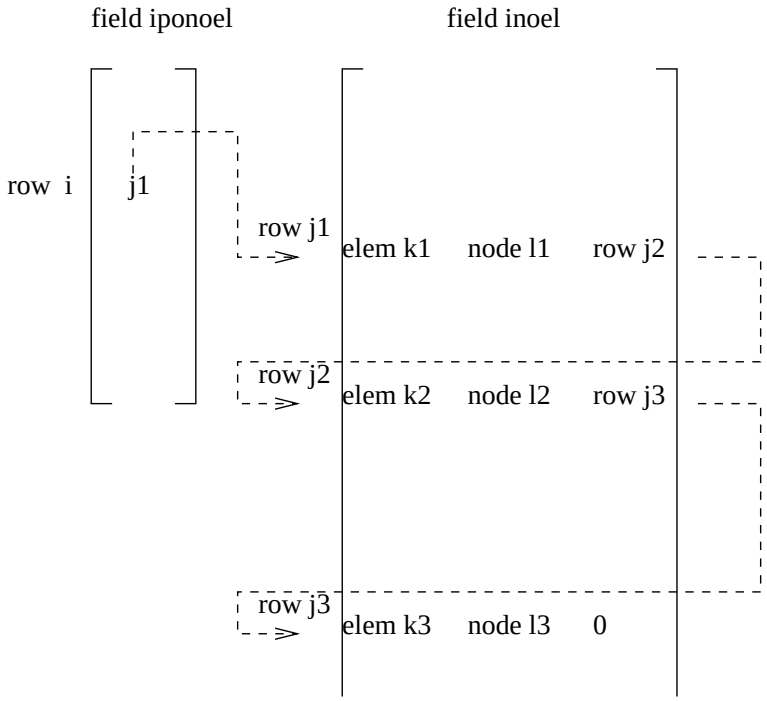


Figure 136: Structures to store all elements to which a given node belongs

9.3.2 Calculating the normals in the nodes

The calculation of the normals (subroutine "gen3dnor.f") in the nodes is performed using a rather complicated algorithm explained in Sections 6.2.13 and 6.2.27. In a node several normals can exist, think for instance of a node on the fold of a roof. Each normal is used to perform an expansion, i.e. in a node with two normals two expansions are performed which partially overlap (Figure 62). Theoretically, as many expansions can be needed as there are elements to which the node belongs to. Therefore, to store the expansions and the normals a structure is used similar to the field kon to store the topology of the elements.

The field kon is a one-dimensional field containing the topology of all elements, one after the other. The entry ipkon(i) points to the location in field kon just before the start of the topology of element i, i.e. the first node of element i is located at position ipkon(i)+1 in field kon, the last node at position ipkon(i)+numnod, where numnod is the number of nodes of the element, e.g. 20 for a 20-node element. Thus, local position m of element j corresponds to global node number kon(ipkon(j)+m). Now, a similar structure is used for the normals and nodes of the expansions since these variables are linked to a local position within an element rather than to a global node number. To this end the two-dimensional field iponor and one-dimensional fields xnor and knor are used.

The entry iponor(1,ipkon(j)+m) points to the location of the normal at local position m of element j within field xnor, i.e. the three components of the normal are stored in xnor(iponor(1,ipkon(j)+m)+1), xnor(iponor(1,ipkon(j)+m)+2) and xnor(iponor(1,ipkon(j)+m)+3). In the same way the entry iponor(2,ipkon(j)+m) points to the location of the new nodes of the expansion at local position m of element j within field knor, i.e. the three new node numbers are stored at knor(iponor(2,ipkon(j)+m)+n), n=1,2,3. The order of the node numbers is illustrated in Figure 61. This applies to the expansion of two-dimensional elements. For the expansion of beam elements xnor contains six entries: three entries for unit vector 1 and three entries for unit vector 2 (Figure 65), i.e. xnor(iponor(1,ipkon(j)+m)+1),...,xnor(iponor(1,ipkon(j)+m)+6). Since the expansion of a beam element leads to 8 extra nodes (Figure 66) 8 entries are provided in field knor. The field xnor is initialized with the values from keyword card *NORMAL.

The procedure runs as follows: for a node i all 2D elements to which the node belongs are determined. Then, the normals on these elements are determined using the procedure explained in Section 6.2.13 starting with the normals predefined by a *NORMAL keyword card. Notice that extra normals are also defined at thickness discontinuities, offset discontinuities or element type changes (e.g. a plane stress element adjacent to a shell element). Therefore, this step is more about how many different expansions are needed rather than different normals: if, for instance the thickness of a flat plate changes discontinuously, two different expansions are needed at the discontinuity nodes although the normal does not change. Next, all beam elements to which node i belongs are determined and normals are determined in a similar way. For each normal appropriate nodes

are generate for the expansion (three for 2D elements, eight for 1D elements). If overall only one normal suffices, no knot exists and no rigid body needs to be defined, unless the rotational degrees of freedom in the node are constrained or moments applied. If more than one normal ensues or the rotational degrees of freedom are addressed by the user in any way, a rigid body is generated. In a rigid body definition all expansion nodes of shells and beam participate, for plane stress, plane strain or axisymmetric elements only the midside nodes take part.

9.3.3 Expanding the 1D and 2D elements

The 1D elements are expanded in subroutine "gen3dfrom1d.f", the 2D elements in "gen3dfrom2d.f".

Expanding the 1D elements involves changing the topology of the element from a 3-node 1D element to a 20-node 3D element using the expanded nodes stored in field knor. Notice that the old node numbers are not used, so at this stage conditions applied to the old node numbers are not yet transferred to the new nodes. To calculate the position of the new nodes the unit vectors 1 and 2, stored in xnor, are used together with the information defined by *BEAM SECTION on the dimensions and the form of the cross section. Both rectangular and elliptical cross sections are allowed.

Expanding the 2D elements requires the thickening of the elements using the expanded node numbers stored in knor and the normals stored in xnor. The element numbers remain, only the topology changes. Notice that the old node numbers are not used, so at this stage conditions applied to the old node numbers are not yet transferred to the new nodes. Plane strain, plane stress and axisymmetric elements require some additional care: these are special elements taking into account specific geometrical configurations. Remember that 8-node 2D elements are expanded into one layer of 20-node brick elements and 6-node 2D elements into one layer of 15-node brick elements. Plane strain, plane stress and axisymmetric elements are defined in one plane, traditionally the x-y plane. Now, for the expansion into 3D this plane is assumed to correspond to z=0. It is the middle plane of the expansion. The elements are expanded half in positive z-direction, half in negative z-direction. Let us call the expanded nodes in positive z-direction the positive-z nodes, the ones in the plane z=0 the zero-z nodes and the rest the negative-z nodes. For plane strain the positive-z and negative-z nodes exhibit exactly the same displacements as the zero-z nodes. These conditions are expressed in the form of multiple point constraints, and are also generated in subroutine "gen3dfrom2d.f". These MPC's greatly reduce the size of the ensuing matrix system. For plane stress elements the positive-z nodes and the negative-z nodes have the same displacements in x- and y-direction as the zero-z nodes. For axisymmetric elements the positive-z nodes and the negative-z nodes have the same displacements as the zero-z nodes for all directions in cylindrical coordinates. Finally, for plane strain, plane stress and axisymmetric elements the displacement in z for the zero-z nodes is zero.

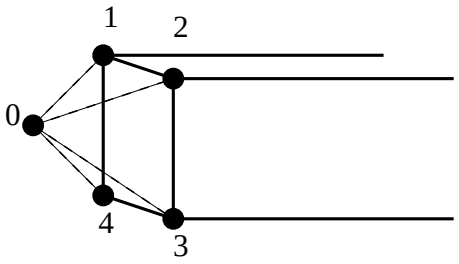


Figure 137: Beam element connection

9.3.4 Connecting 1D and 2D elements to 3D elements

The connection of 1D and 2D elements with genuine 3D elements also requires special care and is performed in subroutine "gen3dconnect.f". Remember that the expanded elements contain new nodes only, so the connection between these elements and 3D elements, as defined by the user in the input deck, is lost. It must be reinstated by creating multiple point constraints. This, however, does not apply to knots. In a knot, a expandable rigid body is defined with the original node as translational node (recall that a knot is defined by a translational, a rotational and an expansion node). Thus, for a knot the connection with the 3D element is guaranteed. What follows applies to nodes in which no knot was defined.

For 1D beam elements the connection is expressed by the equation (see Figure 137 for the node numbers)

$$u_1 + u_2 + u_3 + u_4 - 4u_0 = 0 \tag{381}$$

where u stands for any displacement component (or temperature component for heat transfer calculations), i.e. the above equation actually represents 3 equations for mechanical problems, 1 for heat transfer problems and 4 for thermomechanical problems. Notice that only edge nodes of the beam element are used, therefore it can also be applied to midside nodes of beam elements. It expresses that the displacement in the 3D node is the mean of the displacement in the expanded edge nodes.

For 2D shell elements the connection is expressed by equation (see Figure 138 for the node numbers)

$$u_1 + u_2 - 2u_0 = 0. \tag{382}$$

The same remarks apply as for the beam element.

Finally, for plane strain, plane stress and axisymmetric elements the connection is made according to Figure 139 and equation:

$$u_1 - u_0 = 0. \tag{383}$$

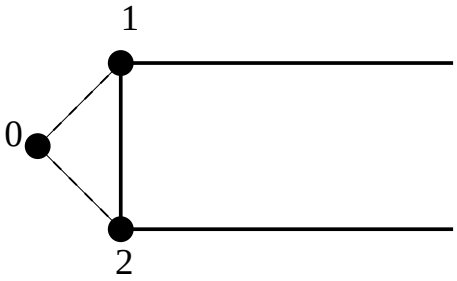


Figure 138: Shell element connection

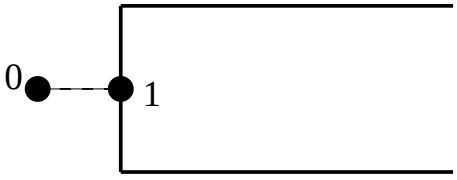


Figure 139: Plane and axisymmetric element connection

Node 1 is the zero-z node of the expanded elements. Although a twenty-node brick element does not use zero-z nodes corresponding the the midside nodes of the original 2D element, they exist and are used in MPC's such as the above equation. The connection is finally established through the combination of the above MPC with the plane strain, plane stress and axisymmetric MPC's linking the zero-z nodes with the negative-z and positive-z nodes.

9.3.5 Applying the SPC's to the expanded structure

Here too, the problem is that the SPC's are applied by the user to the nodes belonging the the original 1D and 2D elements. The expanded nodes, however, have different numbers and a link must be established with the original nodes. This is again performed by multiple point constraints. They are generated in subroutine "gen3dboun.f".

For knots the translational node of the rigid body formulation is the original node number. Consequently, translational SPC's are automatically taken into account. If a rotational SPC is applied, it must be transferred to the rotational node of the knot, e.g. degree of freedom 4 of the original node (rotation about the x-axis) is transformed into degree of freedom 1 of the rotational node.

If no knot is generated in the node to which a translational SPC is applied, the way this node is connected to the newly generated nodes in the expanded elements depends on the type of element. For 1D elements MPC's are generated according to Equation 381 and Figure 137. For 2D shell elements the MPC's correspond to Equation 382 and Figure 138. Finally, for 2D plane and axisymmetric elements the MPC's correspond to Equation 383 and Figure 139.

The application of a rotational SPC to a node in which no knot is defined is performed by generating a mean rotation MPC (cf. Section 8.7.1) about the rotation axis. The rotation axis can be along a global coordinate direction or along a local one. Contrary to translational SPC's, rotational SPC's in a local coordinate system are not converted into MPC's. Rather, the local rotation axis is taken right away as the axis of the mean rotation.

For the temperature degrees of freedom in heat transfer calculations the MPC's generated in beam and shell nodes in which no knot is defined are not sufficient. Indeed, the MPC only specifies the mean of corner nodes (for beams) or the mean of the upper and lower node (for shells). In practice, this corresponds to any bilinear (for beams) or linear (for shells) function across the cross section. In CalculiX, it is not possible to specify this gradient, so a constant function is defined. This is done by assigning the temperature SPC to nodes 2, 3 and 4 (for beams, Equation 381) and to node 2 (for shells, Equation 382).

9.3.6 Applying the MPC's to the expanded structure

The procedure applied here (and coded in subroutine "gen3dmpc.f") is similar to the one in the previous section. The problem consists again of connecting the nodes to which the MPC is applied with the newly generated nodes of the expansion. Each term in the MPC is considered separately. If a knot is defined in the node of the term at stake, nothing needs to be done if a translational degree of freedom is addressed, whereas for a rotational degree of freedom the node is replaced by the rotational node of the knot. If no knot is defined, MPC's satisfying Equation 381 are generated for 1D elements, MPC's satisfying Equation 382 for 2D shell elements and MPC's described by Equation 383 for plane and axisymmetric elements. For the latter elements only the nodes in the zero-z plane are connected, see Figure 139. No rotational degrees of freedom are allowed in nodes of MPC's in which no knot was created.

9.3.7 Applying temperatures and temperature gradients

Temperatures and temperature gradients applied to 1D and 2D elements are transformed into temperatures in the nodes of the expanded elements. To this end the normals and thickness are used to convert the temperature gradients into temperatures in the 3D elements. This is only needed in mechanical calculations with temperature loading. Indeed, in heat transfer calculations the temperatures are unknown and are not applied. Temperature application to 1D and 2D elements is done in subroutine "gen3dtemp.f".

9.3.8 Applying concentrated forces to the expanded structure

This is similar to the application of SPC's: if a knot is defined in the node nothing is done for applied translational forces. For moments (which can be considered as rotational forces) their values are applied to the rotational node of the knot, i.e. the node number is changed in the force application.

If no knot is defined in a node in which a force is applied MPC's are generated between the node at stake and the new nodes in the expanded structure in the case of 1D elements and 2D shells. For 2D plane and axisymmetric elements the force is applied to the zero-z node in the expanded structure. If a moment is applied (only applicable to shells and beams) a mean rotation MPC is generated.

For axisymmetric structures the concentrated forces are assumed to apply for the whole 360°. Since the expansion is done for a small sector only (must be small to keep enough accuracy with only one layer of elements, the size of the sector is specified by the user underneath the *SOLID SECTION card) the force is scaled down appropriately.

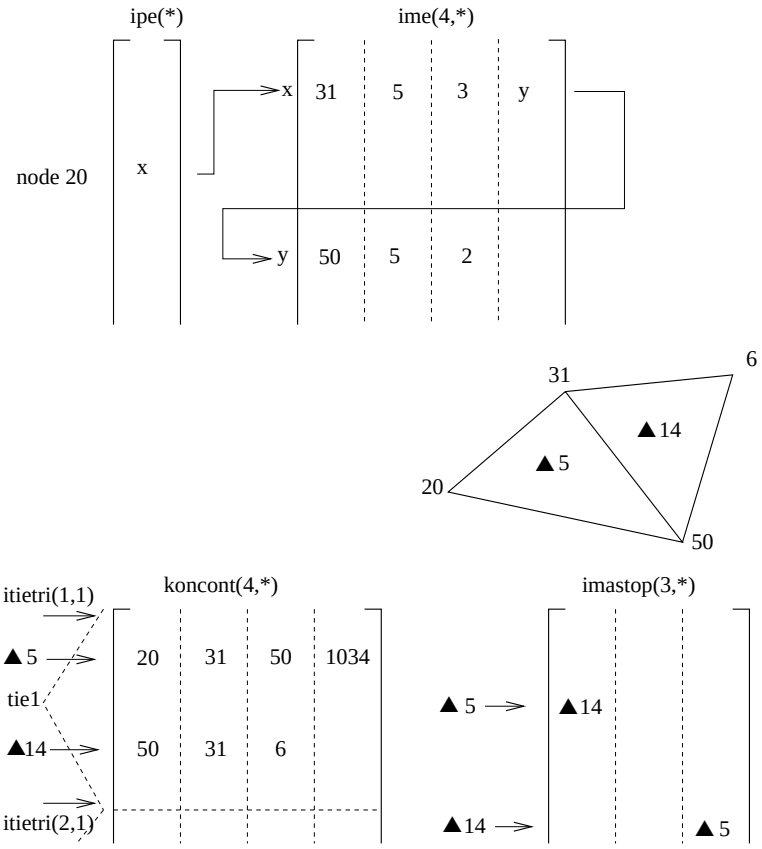
Application of nodal forces is done in subroutine "gen3dforc.f".

9.4 Contact

Contact is triggered by the keyword card *CONTACT PAIR. It defines an interaction between a nodal or element face slave surface and a element face master surface. The master surface is triangulated using standard triangulation schemes for the different kind of faces (3-node, 4-node, 6-node or 8-node). This is done in subroutines allocont.f, triangucont.f and trianeighbor.f. This triangulation is a topological one and does not depend on the concrete coordinates. It is performed at the start of nonlingeo.c. The resulting triangles are stored in field koncont (Figure 140): for triangle i the locations koncont(1..3,i) contain the nodes belonging to the triangle, koncont(4,i) contains the element face to which the triangle belongs. The element face is characterized by a code consisting of 10*(element number)+face number. So the code for face 4 of element 33 is 334. The triangles are stored in the order of the contact tie constraints they belong to. For tie constraint i the location of the first triangle in field koncont is given by itietri(1,i), the location of the last one by itietri(2,i).

The triangulation of the master surfaces allows for fast algorithms to determine the master face opposite of a given slave node. To facilitate this search, a field imastop is created: imastop(i,j) yields for triangle j the triangle opposite of node koncont(i,j). This is the neighboring triangle containing the edge to which node koncont(i,j) does not belong. This adjacency information is needed to apply the search algorithms in Section 1.7 of [24]. To facilitate the construction of imastop (done in subroutine trianeighbor.f), the edges of the triangulation are catalogued by use of two auxiliary fields ipe(*) and ime(4,*). An edge is characterized by two nodes i and j, suppose $i < j$. Then, if no other edge was encountered so far for which i was the lowest node, the present edge is stored in ime(1..4,ipe(i)), where ime(1,ipe(i)) contains j, ime(2,ipe(i)) contains one of the triangles to which the edge belongs, e.g. t1, ime(3,ipe(i)) contains the local position in koncont(1..3,t1) of the node belonging to t1 but not on the edge i-j and ime(4,ipe(i)) is a pointer to ime(1..4,ime(4,ipe(i))) containing any other edge for which i is the lowest node number, else it is zero. 'For node-to-face penalty contact these auxiliary fields are deleted upon leaving trianeighbor. For face-to-face contact they are further used in slavintmortar.f.

For further calculations both the slave nodes and the slave surfaces have to



▲5 belongs to face 4 of element 103

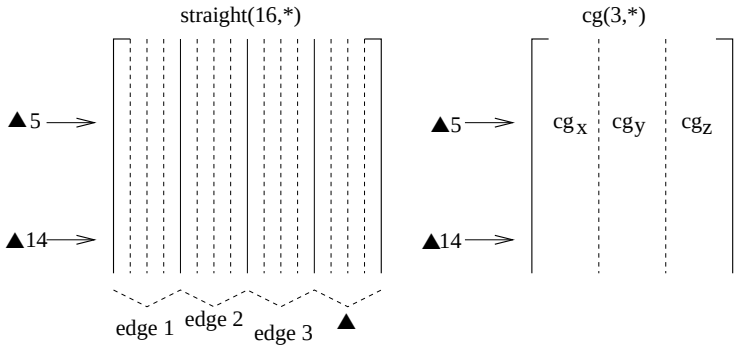


Figure 140: Storage of the triangulation properties

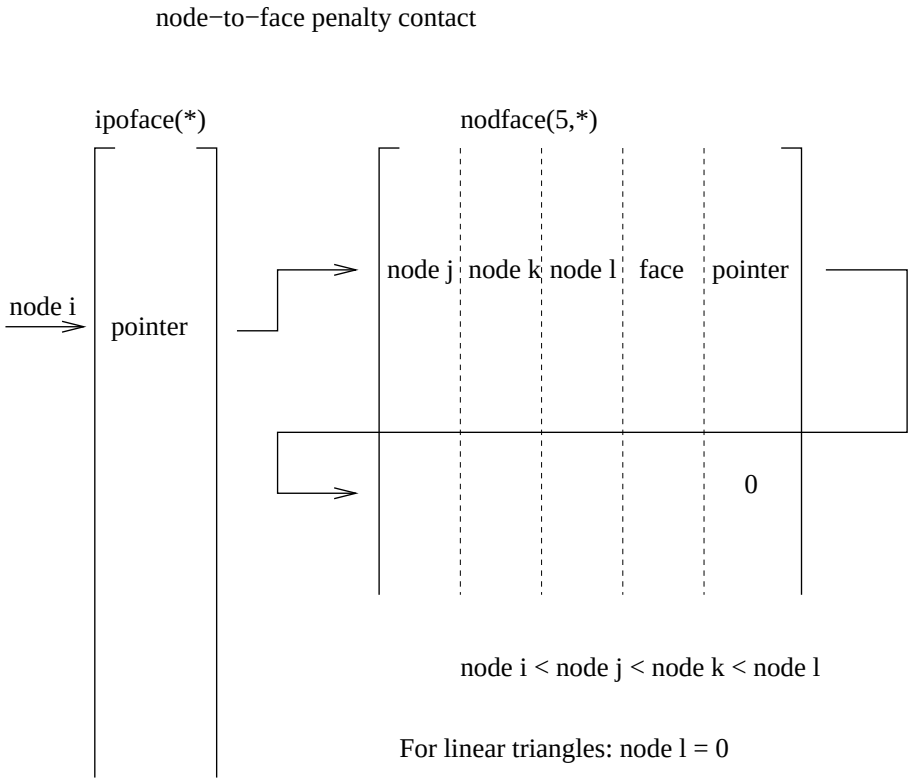


Figure 141: Storage of all faces for the determination of the external faces

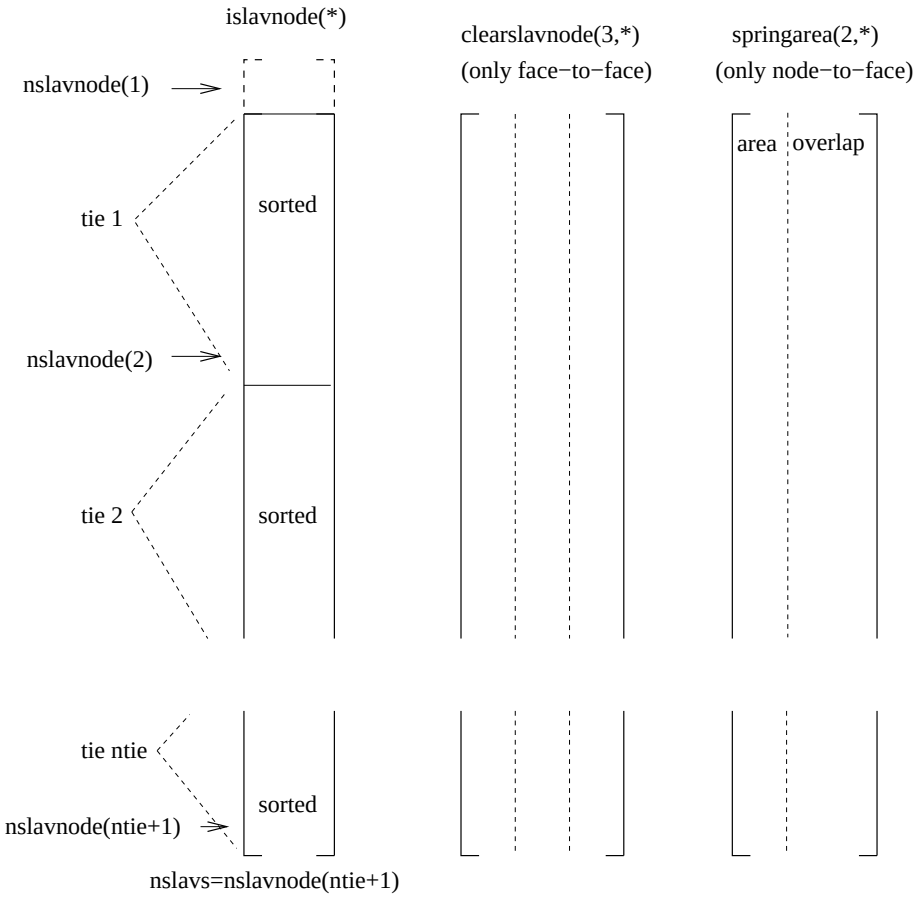


Figure 142: Storage of the slave nodes

be catalogued. In case the slave surface is defined by nodes, the corresponding faces have to be found. To this end, all external faces of the structure are catalogued by fields ipoface and nodface in subroutine findsurface.f (Figure 141). Assuming face f1 to contain corner nodes $i < j < k < l$, f1 is stored in nodface(1..5,ipoface(i)). The entries 1..5 contain: node j, node k, node l, a face label in the form 10*element number + local face number and a pointer to any other face for which i is the lowest node.

The slave nodes are stored in field islavnode(*) (Figure 142), tie per tie and sorted in increasing order for each tie separately. nslavnode(i) contains the position in islavnode before the first slave node of tie i. If ntie is the number of ties, nslavnode contains ntie+1 entries, in order to mark the end of the field islavnode as well. The total number of slave nodes is denoted by nslavs. For face-to-face contact the field clearslavnode contains the difference between the clearance specified by the user with the keyword card *CLEARANCE and the

clearance calculated based on the actual coordinates. This field is zero in the absence of the *CLEARANCE card. The field clearini contains the clearance for each node belonging to the slave face at stake. This information is copied from field clearslavnode.

The slave faces are stored in islavsurf(1..2,*) (Figure 143 and Figure 144). islavsurf(1,*) contains the slave faces, tie per tie (not in any way sorted), whereas islavsurf(2,*) is an auxiliary field not further needed for node-to-face contact. itiefac(1,i) is a pointer into field islavsurf marking the first face for tie i, itiefac(2,i) points to the last face. The total number of slave faces is ifacecount. The area of the slave faces is stored in a corresponding field areaslav. For face-to-face contact the second column of islavsurf is used as a pointer to locations in field pslavsurf, preceding the integration points in the face (local coordinates and weights). If for a given integration point in the slave face an opposite master face is found, the local coordinates, the label of the master face and the local normal to the master face are stored in field pmastsurf.

For the purpose of calculating the area corresponding to a given slave node, the fields iponoels and inoels are used (Figure 145). For a slave node i, the value iponoels(i) points towards an entry inoels(1..3,iponoels(i)) containing the position within field islavsurf(1,*) of a face to which node i belongs and an entry inoels(2,iponoels(i)) pointing to any other faces to which node i belongs. Field xnoels contains the weight of the node within the face. This information is gathered in subroutine inicont.c.

The master nodes are catalogued in field imastnode in the sane way that the slave nodes are stored in islavnode (Figure 146). The master nodes are stored tie per tie, within each tie they are sorted in ascending order. For tie i nmastnode(i) points towards the location in imastnode immediately before the master node with the smallest number within tie i, nmastnode(i) points towards the master node within tie i with the largest number. The size of imastnode is nmastnode(ntie+1), where ntie is the number of ties. In each iteration and/or increment the topological information of each master triangle is complemented by geometrical information consisting of the center of gravity (in field cg) and the equations of the triangle plane and the planes quasi-perpendicular to the triangle and containing its edges. For triangle i the coordinates of the center of gravity are stored in cg(1..3,i). The coefficients of the equation of the plane orthogonal to the triangle and containing the first edge are stored in straight(1..4,i). The first edge is defined as the edge through nodes koncont(1,i) and koncont(2,i). Similar for edge 2 (straight(5..8,i)) and edge 3 (straight(9..12,i)). The coefficients of the triangle plane are stored in straight(13..16,i). The geometrical information is calculated in routine updatecontpen.f. The planes bordering the triangles are quasi-orthogonal to the triangle in the sense that they are inbetween the truly orthogonal planes and the planes through the triangle edges and orthogonal to the neighboring triangles. To this end the mean normals are stored in field xmastnor(3,*) (Figure 146).

Further geometrical information is the area of each slave face i, stored in areaslav(i), the area corresponding to slave node i, stored in springarea(1,i) and the penetration at the start of each step in slave node i (< 0 if any penetration

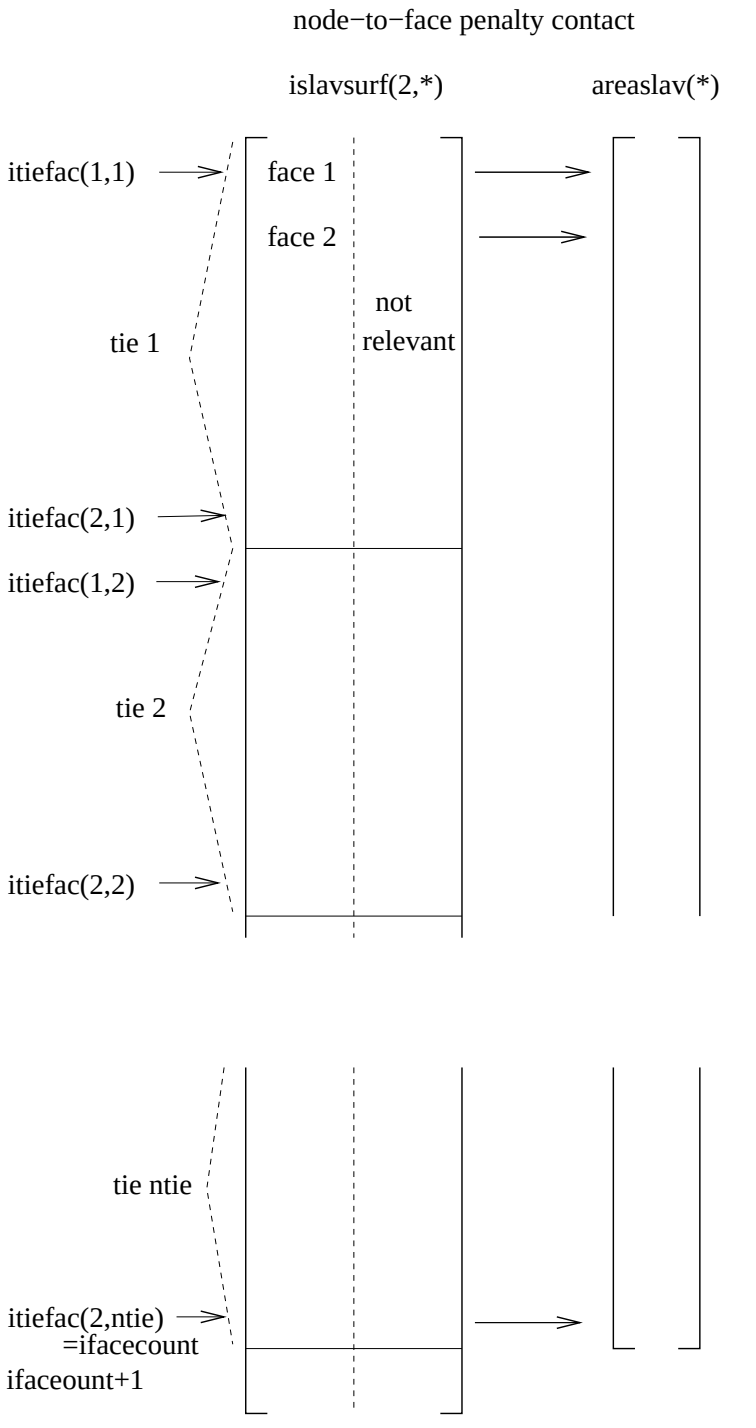


Figure 143: Storage of the slave faces (node-to-face penalty)

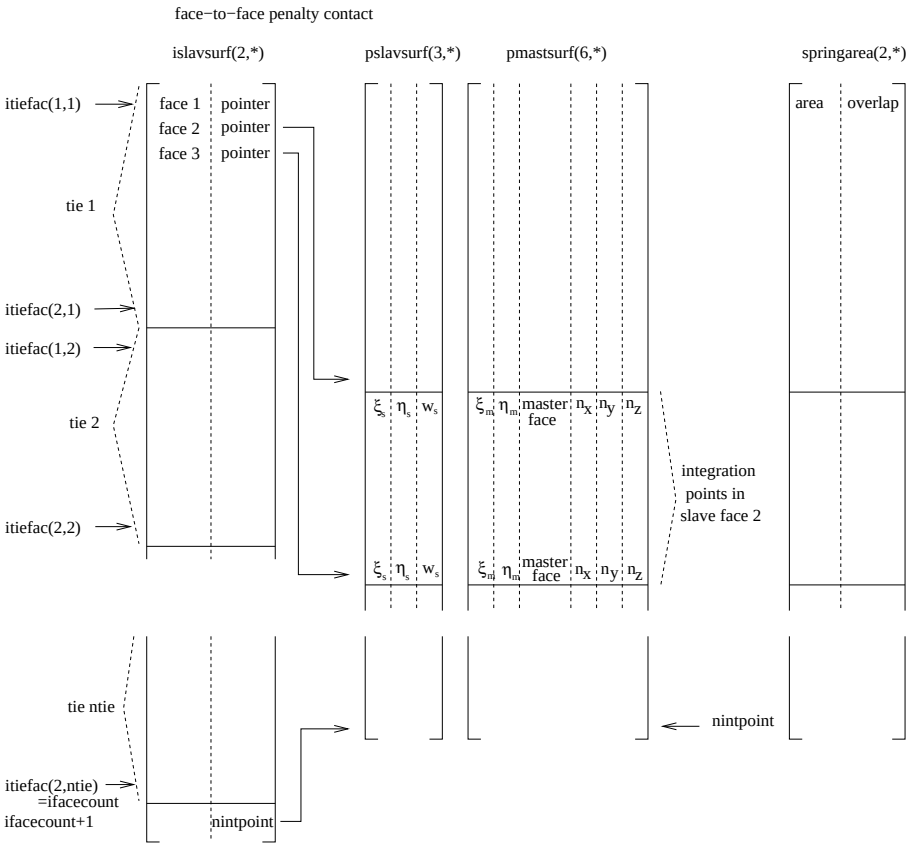


Figure 144: Storage of the slave faces (face-to-face penalty)

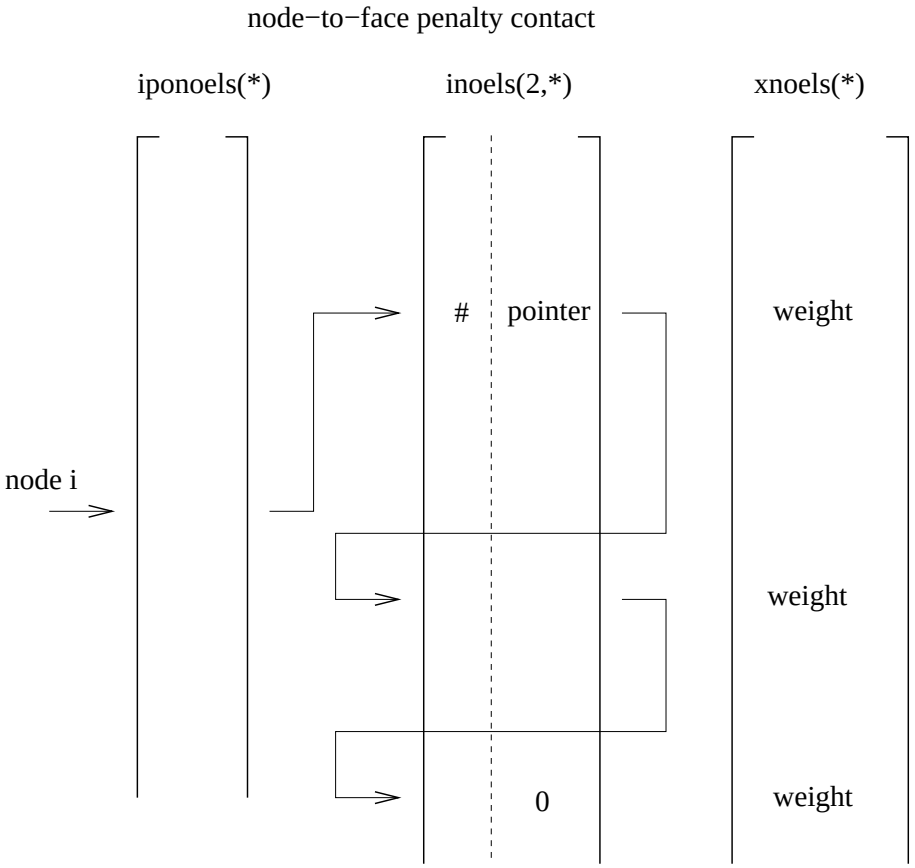


Figure 145: Storage of the slave faces belonging to a given slave node

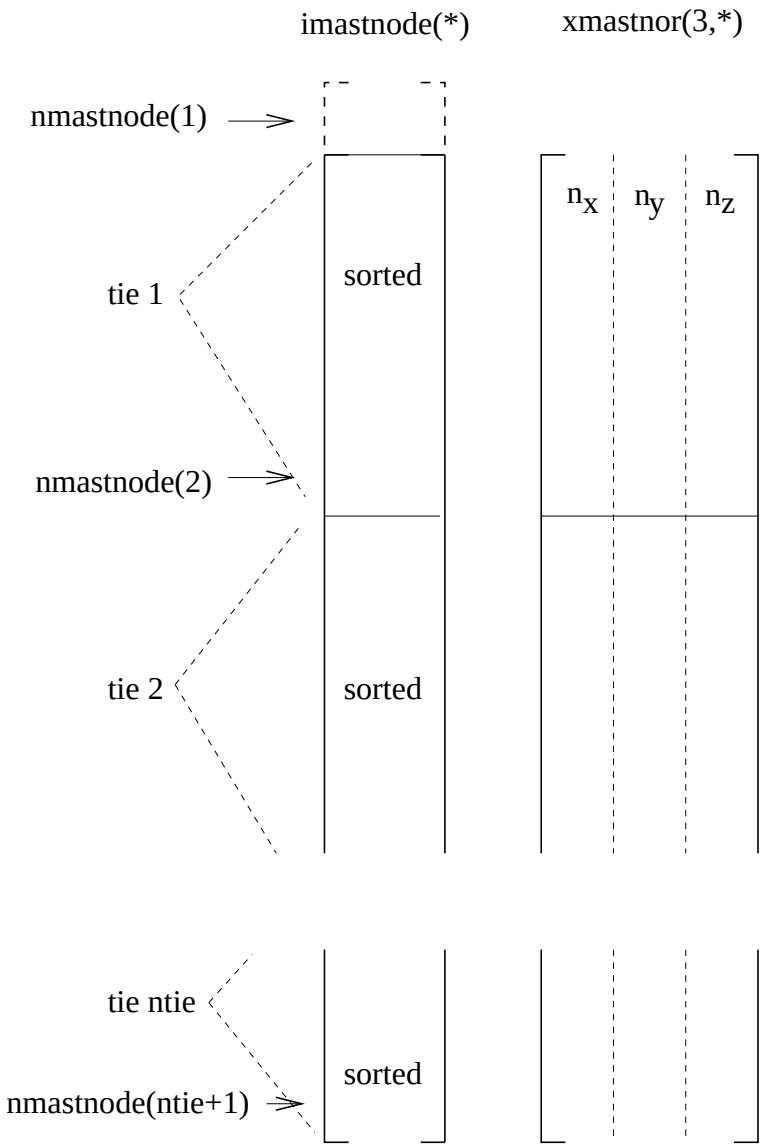


Figure 146: Storage of the master nodes

, else 0), stored in springarea(2,i). These calculations are performed each time gencontelem_n2f.f or gencontelem_f2f.f is called.

Subsequently, contact spring elements are generated (routine gencontelem.f). To this end, each node belonging to the dependent contact slave surface is treated separately. To determine the master surface the node interacts with, a triangle belonging to the triangulation of the corresponding master surface are identified, such that its center of gravity is closest to the dependent node. Then, a triangle is identified by adjacency, such that the orthogonal projection of the slave node is contained in this triangle. If such a triangle is found, a contact spring element is generated consisting of the dependent node and the independent surface the triangle belongs to, provided the node penetrates the structure or the clearance does not exceed a given margin. Before checking the penetration or clearance an adjustment of the geometry is performed in case the user has activated the ADJUST parameter. If any of these conditions is not satisfied, no contact spring element is generated for this dependent node and the next node is treated. The sole purpose of the triangulation of the master surface is the fast identification of the independent face a dependent node interacts with.

The stiffness matrix of the contact spring elements is calculated in springstiff.f, called by mafillsm.f. In order to determine the stiffness matrix the local coordinates of the projection of the dependent node onto the independent surface are needed. This is performed in attach.f. Use is made of a cascaded regular grid to determine the location within the independent surface which is closest to the dependent node. The local coordinates are needed to determine the shape functions and their derivatives. The contact force is determined in springforc.f, called by results.f. Here too, routine attach.f is called.

Since the geometrical information is recalculated in every iteration, large deformations are taken into account, unless the user has specified SMALL SLIDING in which case the geometry update takes place once at the start of each new increment.

The material properties of the contact spring, defined by means of the *SURFACE INTERACTION, the *SURFACE BEHAVIOR and the *FRICTION card, are stored in the same fields as the *MATERIAL and *ELASTIC,TYPE=ISOTROPIC card.

The general structure of the contact algorithms for nonlinear geometric calculations is as follows. The contact topology is determined in inicont.c. This routine is called once at the start of a new step and calls the following routines:

- allocont: determining the number of master triangles and slave entities (nodes or faces, depending on whether the slave surface is nodal or facial)
- triangucont: triangulation of the master side
- trianeighbor: determining the triangle neighbors in the triangulation of the master side
- findsurface (only for node-to-face contact): catalogueing the external faces and creating the fields ipoface and nodface

- tiefaccont: determinnig the field islavsurf and itieface (slave nodes), islavnode and nslavnode (slave faces), iponoels, xnoels and inoels (only for node-to-face contact) and imastnode and nmastnode (master nodes).

For face-to-face contact the routine precontact.c is called at the start of each new increment. Its purpose is:

- to calculate the center of gravity and the quasi-orthogonal planes to the master triangles (updatecontpen.f).
- to calculate the clearance (if the *CLEARANCE keyword card is used) and/or adjust the slave nodes (if the ADJUST parameter is used on the *CONTACT PAIR card) at the start of the first step (adjustcontactnodes.f).
- to determine the location of the integration points in the slave faces based on the matching of the slave and the master faces (slavintpoints.f).

Furthermore, for face-to-face contact the routine interpolatestate is called at the start of each new increment. It interpolates the state variables (internal variables such as the slip accumulated so far) from the integration points at the end of the previous increment, if any, to the new integration points determined in slavintpoints.f. Indeed, at the start of a new increment the matching between the slae and master surfaces is done anew and usually leads to a change in the location of the integration points.

The contact.c routine is called once per iteration. This applies to node-to-face as well as face-to-face contact. For node-to-face contact the purpose of contact.c is:

- to update the center of gravity and the quasi-orthogonal planes of the master triangles (updatecontpen.f).
- to generate contact spring elements at those slave nodes for which the clearance does not exceed a predefined value c_0 (gencontelem_n2f.f). Additionally, gencontelem_2nf performs the calculation of:
  - the area of all slave faces (stored in areaslav).
  - the area corresponding to each slave node and the overlap at the start of the first step (stored in springarea).

If a spring element is generated, its topology is stored in field kon in accordance to Figure 147. The parameter iloc is needed to identify the area and overlap.

For face-to-face contact contact.c only calls routine gencontelem_f2f. At the start of a new increment the field pmastsurf is filled for those slave integration points for which an opposite master face is found. It contains the local coordinates of the master face, its label (10*element+local face number) and

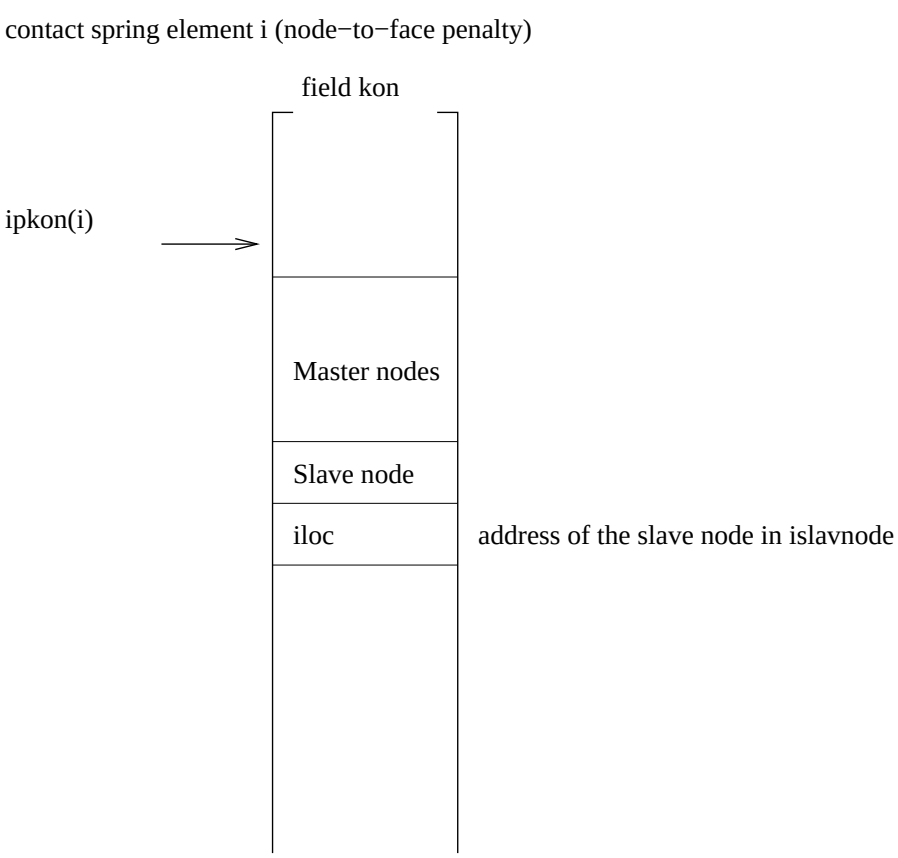


Figure 147: Topology of the node-to-face contact elemetns

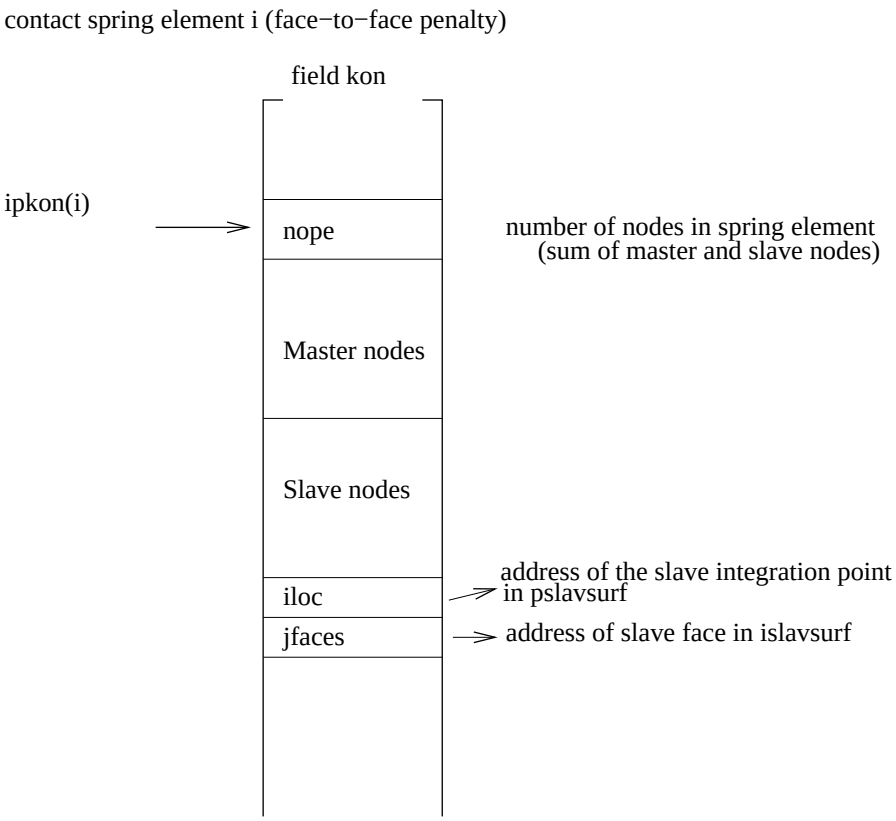


Figure 148: Topology of the face-to-face contact elements

the local normals. Furthermore, field springarea is filled containing the corresponding slave area and the overlap at the start of each increment in the first step. Please note that pmastsurf and springarea are calculated at the start of an increment and kept constant for all iterations across the complete increment. The contact spring elements, however, are generated anew in each iteration based on the sign of the clearance. A contact element is generated only if the clearance is negative (i.e. in case of penetration). The topology of the spring element is stored in field kon (Figure 148) and contains the total number of nodes (slave+master), the master nodes, the slave nodes, the address of the integration point in pslavsurf and the address of the slave face in islavsurf.

9.5 Determining the matrix structure

This part consists of the following subparts:

- matching the SPC's
- de-cascading the MPC's
- renumbering the nodes to decrease the profile
- determining the matrix structure

9.5.1 Matching the SPC's

In each step the SPC's can be redefined using the OP=NEW parameter. To assure a smooth transition between the values at the end of the previous step and the newly defined values these must be matched. This matching is performed in subroutine spcmatch.f. For each SPC i active in a new step the following cases arise:

- a SPC j in the same node and in the same direction was also active in the previous step; this SPC is identified and the corresponding value, which was stored in position j of field xbounold before calling spcmatch, is now stored in position i of field xbounold.
- in the previous step no corresponding SPC (i.e. in the same direction in the same node) was applied. The appropriate displacement value at the end of the previous step is stored in position i of field xbounold.

9.5.2 De-cascading the MPC's

Multiple point constraints can depend on each other. For instance:

$$5.u_1(10) + 8.u_1(23) + 2.3u_2(12) = 0 \tag{384}$$

$$u_1(23) - 3.u_1(2) + 4.u_1(90) = 0 \tag{385}$$

The first equation depends on the second, since $u_1(23)$ belongs to the independent terms of the first equation, but it is the dependent term in the second (the first term in a MPC is the dependent term and is removed from the global system, the other terms are independent terms). Since the dependent terms are removed, it is necessary to expand ("de-cascade", since the equations are "cascaded" like falls) the first equation by substituting the second in the first, yielding:

$$5.u_1(10) + 24.u_1(2) - 32.u_1(90) + 2.3u_2(12) = 0 \tag{386}$$

This is done in subroutine cascade.c at least if the MPC's which depend on each other are linear. Then, the corresponding terms are expanded and the MPC's are replaced by their expanded form, if applicable.

However, the expansion is not done if any of the MPC's which depend on each other is nonlinear. For nonlinear MPC's the coefficients of the MPC are not really known at the stage in which cascade.c is called. Indeed, in most cases the coefficients depend on the solution, which is not known yet: an iterative procedure results. Therefore, in a nonlinear MPC terms can vanish during the solution procedure (zero coefficients) thereby changing the dependencies between the MPC's. Thus, the dependencies must be determined in each iteration anew and subroutine cascade.c is called from within the iterative procedure in subroutine nonlingeo.c. This will be discussed later.

In cascade.c there are two procedures to de-cascade the MPC's. The first one (which is the only one productive right now) is heuristic and iteratively expands the MPC's until no dependencies are left. This procedure worked very well thus far, but lacks a theoretical convergence proof. The second procedure, which is assured to work, is based on linear equation solving and uses SPOOLES. The dependent terms are collected on the left hand side, the independent ones on the right hand side and the sets of equations resulting from setting one independent term to 1 and the others to 0 are subsequently solved: the system of equations

$$\left[A\right]\left\{U_d\right\} = \left[B\right]\left\{U_i\right\} \tag{387}$$

is solved to yield

$$\left\{U_d\right\} = \left[A\right]^{-1}\left[B\right]\left\{U_i\right\} \tag{388}$$

in which $\left[U_d\right]$ are the dependent terms and $\left[U_i\right]$ the independent terms. However, in practice the MPC's do not heavily depend on each other, and the SPOOLES procedure has proven to be much slower than the heuristic procedure.

9.5.3 Renumbering the nodes to decrease the profile

The profile of a matrix is obtained by marking in each column the uppermost nonzero entry. This way one gets a kind of skyscraper picture. Reducing the profile as much as possible by renumbering the nodes usually speeds up the solution of the equation system. This is done using an algorithm published by

Sloan ([70]) in subroutine renumber.f. It not only takes the topology of the elements into account, it can also take care of additional equations introduced by *EQUATION or *MPC statements. Although it is primarily effective when using a profile solver [78], it seems to have a beneficial effect on the solver time of SPOOLES as well. Therefore, it is always activated.

9.5.4 Determining the matrix structure.

This important task is performed in mastruct.c for structures not exhibiting cyclic symmetry and mastructcs.c for cyclic symmetric structures. Let us focus on matruct.c.

The active degrees of freedom are stored in a two-dimensional field nactdof. It has as many rows as there are nodes in the model and four columns since each node has one temperature degree of freedom and three translational degrees. Because the 1-d and 2-d elements are expanded into 3-d elements in routine "gen3delem.f" there is no need for rotational degrees of freedom. In C this field is mapped into a one-dimensional field starting with the degrees of freedom of node 1, then those of node 2, and so on. At first, all entries in nactdof are deactivated (set to zero). Then they are (de)activated according to the following algorithm:

- In a mechanical or a thermomechanical analysis the translational degrees of freedom of all nodes belonging to elements are activated.
- In a thermal or a thermomechanical analysis the temperature degree of freedom of all nodes belonging to elements are activated.
- All degrees of freedom belonging to MPC's are activated (dependent and independent)
- The degrees of freedom corresponding to SPC's are deactivated
- The degrees of freedom corresponding to the dependent side of MPC's are deactivated.

Then, the active degrees of freedom are numbered. Subsequently, the structure of the matrix is determined on basis of the topology of the elements and the multiple point constraints.

For SPOOLES, ARPACK and the iterative methods the storage scheme is limited to the nonzero SUBdiagonal positions of the matrix only. The scheme is as it is because of historical reasons, and I do not think there is any reason not to use another scheme, such as a SUPERdiagonal storage. The storage is described as follows:

- the field irow contains the row numbers of the SUBdiagonal nonzero's, column per column.
- icol(i) contains the number of SUBdiagonal nonzero's in column i.

- jq(i) contains the location in field irow of the first SUBdiagonal nonzero in column i

All three fields are one-dimensional, the size of irow corresponds with the number of nonzero SUBdiagonal entries in the matrix, the size of icol and jq is the number of active degrees of freedom. The diagonal entries of the matrix stored separately and consequently no storage information for these items is needed.

The thermal entries, if any, are stored after the mechanical entries, if any. The number of mechanical entries is neq[0] (C-notation), the total number of entries (mechanical and thermal) is neq[1]. In the same way the number of nonzero mechanical SUBdiagonal entries is nzs[0], the total number of SUBdiagonal entries is nzs[1]. In thermomechanical applications the mechanical and thermal sub-matrices are assumed to be distinct, i.e. there is no connection in the stiffness matrix between the mechanical and the thermal degrees of freedom. Therefore, the mechanical and thermal degrees of freedom occupy two distinct areas in the storage field irow.

File mastructcs calculates the storage for cyclic symmetric structures. These are characterized by the double amount of degrees of freedom, since cyclic symmetry results in a complex system which is reduced to a real system twice the size. The cyclic symmetry equations are linear equations with complex coefficients and require a separate treatment. The fields used for the storage, however, are the same.

9.6 Filling and solving the set of equations, storing the results

In this section a distinction is made between the types of analysis and the solver used:

- for linear static calculations with SPOOLES or the iterative solver the appropriate routine is prespooles.c
- for nonlinear static or dynamic calculations (which implies the use of SPOOLES or the iterative solver) routine nonlingeo.c is called. This includes all thermal calculations.
- for frequency analysis without cyclic symmetry routine arpack.c is called.
- for a frequency analysis with cyclic symmetry conditions the appropriate routine is arpackcs.c
- for a buckling analysis arpackbu.c is called
- for linear dynamic calculations (i.e. modal dynamic analysis) the routine is dyna.c
- finally, for steady state dynamics calculations the routine is steadystate.c

9.6.1 Linear static analysis

For a linear static analysis (prespooles.c) the structure is as follows:

- determine the loads at the end of the step in routine tempload.f
- fill the matrix (routine mafillsm)
- solve the system of equations (routines spooles or preiter)
- determine the required results for all degrees of freedom, starting from the displacement solution for the active degrees of freedom. This is done in subroutine results.f, including any storage in the .dat file.
- store the results in the .frd file. For structures not exhibiting cyclic symmetry this is performed in routine out.f, for cyclic symmetric structures routine frdcyc.c is called before calling out. If an error occurred during the matrix fill the output is reduced to the pure geometry.

The different routines in the above listing will be discussed separately, since they are common to most types of analysis.

9.6.2 Nonlinear calculations

For nonlinear calculations the solution is found by iteration. Because a step is possibly too large to obtain convergence, the option exists to subdivide the step into a finite number of increments. The size of the initial increment in a step is defined by the user (line beneath *STATIC, *DYNAMIC, *VISCO, *HEAT TRANSFER or *COUPLED TEMPERATURE-DISPLACEMENTS) and also the number of increments can be controlled by the user (parameter DIRECT). However, in most cases it is advisable to let the program determine the size of the increments, based on the convergence rate of the previous increments. The solution in each increment is obtained by iteration until the residual forces are small enough.

Therefore, the structure of nonlingeo corresponds to the flow diagram in Figure 149. It lists all subroutines, each line is a subroutine. On the upper right "preliminary" is an abbreviation for five subroutines which recur often. If a subroutine or a group of subroutines is enclose by square brackets, it means that it is only run under certain conditions. In detail, the structure of nonlingeo looks like:

- before the first increment
  - determine the number of advective degrees of freedom and the number of radiation degrees of freedom (envtemp.f)
  - expanding the radiation degrees of freedom in case of cyclic symmetry (radcyc.c)
  - initialization of contact fields and triangulation of the independent contact surfaces (inicont.c)

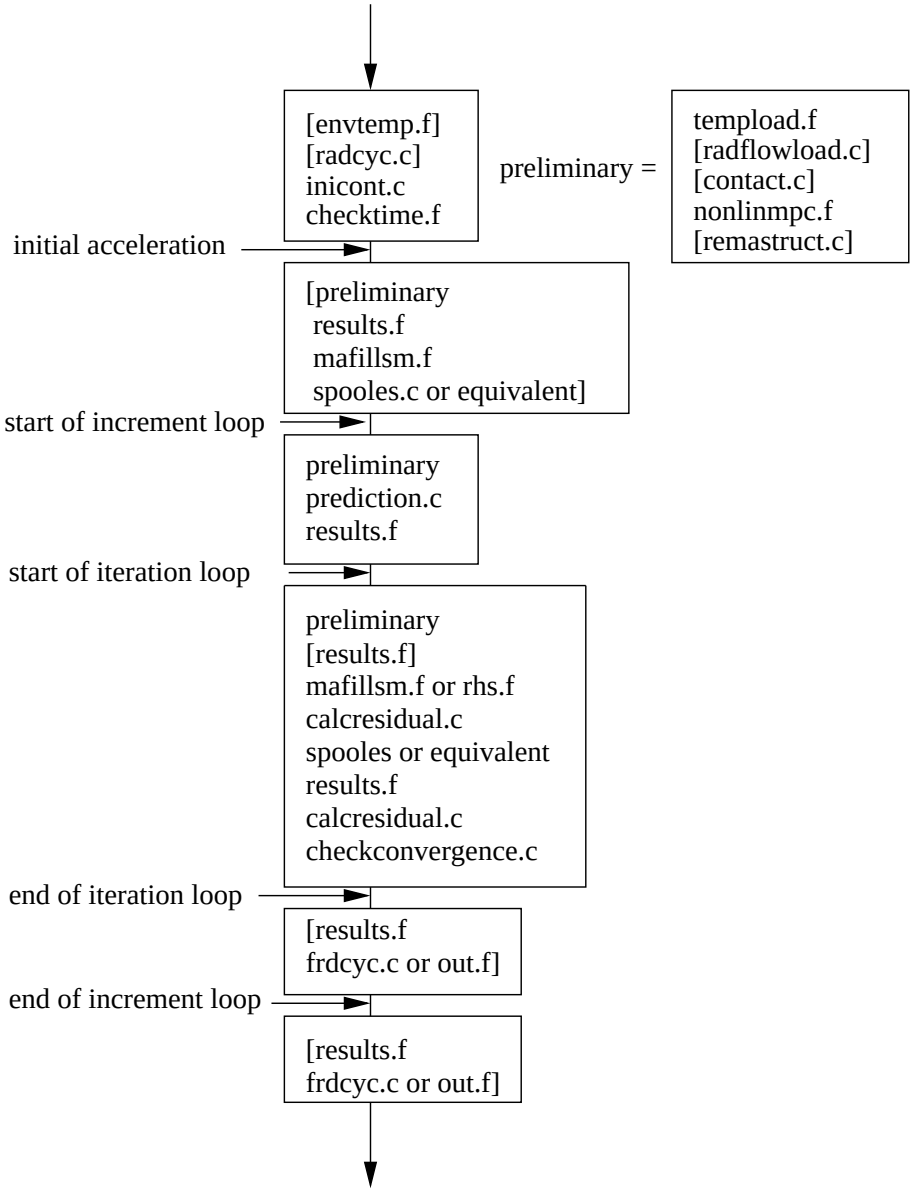


Figure 149: Flow diagram for subroutine nonlingeo

  - take into account time point amplitudes, if any (checktime.f).
  - calculate the initial acceleration and the mass matrix (specific heat matrix for transient heat transfer calculations) for dynamic calculations. (initialaccel.c). This includes:
    * determine the load at the start of the increment (tempload.f)
    * for thermal analyses: determine the sink temperature for forced convection and cavity radiation boundary conditions (radflowload.f)
    * update the location of contact and redefine the nonlinear contact spring elements (contact.f)
    * update the coefficients of nonlinear MPC's, if any.
    * if the topology of the MPC's changed (dependence of nonlinear MPC's on other linear or nonlinear ones) or contact is involved: call remastruct
    * determine the internal forces (results.f).
    * construction of the stiffness and mass matrix and determination of the external forces (mafillsm.f); This is also done for explicit calculations in order to get the mass matrix.
    * subtract the internal from the external forces to obtain the residual forces;
    * solving the system of equations with in spooles.c, preiter.c or any other available sparse matrix solver. For explicit dynamic calculations explicit calculation of the solution (no system needs to be solved). The solution is the acceleration at the start of the step.

- for each increment
  - before the first iteration
    * determine the load at the end of the increment (tempload.f)
    * for thermal analyses: determine the sink temperature for forced convection and cavity radiation boundary conditions (radflowload.f)
    * update the location of contact and redefine the nonlinear contact spring elements (contact.f)
    * update the coefficients of nonlinear MPC's, if any.
    * if the topology of the MPC's changed (dependence of nonlinear MPC's on other linear or nonlinear ones) or contact is involved: call remastruct.
    * prediction of the kinematic vectors
    * determination of the internal forces (results.f). The difference between the internal and the external forces are the residual forces. If the residual forces are small enough, the solution is found. If they are not, iteration goes on until convergence is reached. The residual forces are the driving forces for the next iteration.

  - in each iteration
    * determine the load at the end of the increment (tempload.f)
    * for thermal analyses: determine the sink temperature for forced convection and cavity radiation boundary conditions (radflowload.f)
    * update the location of contact and redefine the nonlinear contact spring elements (contact.f)
    * update the coefficients of nonlinear MPC's, if any.
    * if the topology of the MPC's changed (dependence of nonlinear MPC's on other linear or nonlinear ones) or contact is involved: call remastruct and redetermine the internal forces (results.f).
    * construct the system of equations and determination of the external forces (mafillsm.f); for explicit dynamic calculations no system has to be set up, only the external forces are determined (rhs.f).
    * subtract the internal from the external forces to obtain the residual forces (calcresidual.c);
    * solving the system of equations with in spooles.c, preiter.c or any other available sparse matrix solver. For explicit dynamic calculations explicit calculation of the solution (no system needs to be solved).
    * calculating the internal forces and material stiffness matrix in each integration point in results.f
    * deriving the new residual by subtracting the updated internal forces from the external forces (calcresidual.c).
    * If the residual is small enough iteration ends (checkconvergence.c). The convergence criteria are closely related to those used in ABAQUS.
  - after the final iteration, if output was not suppressed by user input control:
    * determining the required results for all degrees of freedom, starting from the displacement solution for the active degrees of freedom. This is done in subroutine results.f, including any storage in the .dat file.
    * storing the results in the .frd file. For structures not exhibiting cyclic symmetry this is performed in routine out.f, for cyclic symmetric structures routine frdcyc.c is called before calling out. If an error occurred during the matrix fill the output is reduced to the pure geometry.

- after the final increment (only if no output resulted in this final increment due to user input control)
  - determining the required results for all degrees of freedom, starting from the displacement solution for the active degrees of freedom.

This is done in subroutine results.f, including any storage in the .dat file.

– storing the results in the .frd file. For structures not exhibiting cyclic symmetry this is performed in routine out.f, for cyclic symmetric structures routine frdcyc.c is called before calling out. If an error occurred during the matrix fill the output is reduced to the pure geometry.

9.6.3 Frequency calculations

Frequency calculations are performed in subroutines arpack.c for structures not exhibiting cyclic symmetry and arpackcs.c for cyclic symmetric structures. Frequency calculations involve the following steps:

- filling the stiffness and mass matrix in mafillsm.f. The stiffness matrix depends on the perturbation parameter: if iperturb=1 the stress stiffness and large deformation stiffness of the most recent static step is taken into account ([18])
- solving the eigenvalue system using SPOOLES and ARPACK
- calculating the field variables in results.f, including storing in the .dat file
- storing the results in .frd format in out.f

The eigenvalues and eigenmodes are solved in shift-invert mode. This corresponds to Mode 3 in ARPACK ([41]). Suppose we want to solve the system

$$\left[K\right]\left\{U\right\} = \omega^2 \left[M\right]\left\{U\right\} \tag{389}$$

then the shift-invert mode requires algorithms for solving

$$\left[K - \sigma M\right]\left\{U\right\} = \left\{X_1\right\} \tag{390}$$

and for calculating

$$\left\{Y\right\} = \left[M\right]\left\{X_2\right\} \tag{391}$$

where $\left\{X_1\right\}$ and $\left\{X_2\right\}$ are given and σ is a parameter. In CalculiX, it is set to 1. These operations are used in an iterative procedure in order to determine the eigenvalues and the eigenmodes. For the first operation SPOOLES is used. SPOOLES solves a system by using a LU decomposition. This decomposition is performed before the iteration loop initiated by ARPACK since the left hand side of Equation (390) is always the same. Only the backwards substitution is inside the loop. The second operation (Equation (391)) is performed in routine op.f and is a simple matrix multiplication. Notice that this routine depends on the storage scheme of the matrix.

For cyclic symmetric structures the following additional tasks must be performed:

- Expanding the structure in case more than one segment is selected for output purposes (parameter NGRAPH on the *CYCLIC SYMMETRY MODEL keywork card). This is done before the mafillsm call.
- Calculating the results for the extra sectors based on the results for the basis sector. This is performed after the call of routine results.f.

9.6.4 Buckling calculations

To calculate buckling loads routine arpackbu.c is called. The following steps are needed in a buckling calculation:

- calculation of the stresses due to the buckling load. This implies setting up the equation system in mafillsm.f, solving the system with SPOOLES and determining the stresses in results.f
- setting up the buckling eigenvalue system consisting of the stiffness matrix $\left[K\right]$ of the previous static step (including large deformation stiffness and stress stiffness) and the stress stiffness matrix $\left[KG\right]$ of the buckling load [18].
- loop with starting value for $\sigma = 1$
  - LU decomposition of $\left[K - \sigma KG\right]$
  - iterative calculation of the buckling factor with ARPACK
  - determination of the buckling mode
  - if $5\sigma <$ buckling factor $< 50000\sigma$ exit loop, else set $\sigma =$ buckling factor$/500$ and cycle
- determine the stresses and any other derived fields

The buckling mode in ARPACK (Mode 4, cf [41]) is used to solve a system of the form

$$\left[K\right]\left\{U\right\} = \lambda\left[KG\right]\left\{U\right\} \tag{392}$$

where $\left[K\right]$ is symmetric and positive definite and $\left[KG\right]$ is symmetric but indefinite. The iterative procedure to find the eigenvalues requires routines to solve

$$\left[K - \sigma KG\right]\left\{U\right\} = \left\{X_1\right\} \tag{393}$$

and to calculate

$$\left\{Y\right\} = \left[K\right]\left\{X_2\right\}. \tag{394}$$

Similar to the frequency calculations, the LU decomposition (SPOOLES) to solve Equation (393) is performed before the loop determining the buckling

factor, since the left hand side of the equation does not vary. The matrix multiplication in Equation (394) is taken care of by routine op.f.

A major difference with the frequency calculations is that an additional iteration loop is necessary to guarantee that the value of the buckling factor is right. Indeed, experience has shown that the value of σ matters here and that the inequality $5\sigma <$ buckling factor $< 50000\sigma$ should be satisfied. If it is not, the whole procedure starting with the LU decomposition is repeated with a new value of $\sigma =$ buckling factor/500. If necessary, up to four such iterations are allowed.

9.6.5 Modal dynamic calculations

For modal dynamic calculations the response of the system is assumed to be a linear combination of the lowest eigenmodes. To this end, the eigenvalues and eigenmodes must have been calculated, either in the same run, or in a previous run. At the end of a frequency calculation this data, including the stiffness and mass matrix, is stored in binary form in a .eig file, provided the STORAGE=YES option is activated on the *FREQUENCY or *HEAT TRANSFER,FREQUENCY card. This file is read at the beginning of file dyna.c.

In file dyna.c the response is calculated in an explicit way, for details the reader is referred to [18]. Modal damping is allowed in the form of Rayleigh damping. Within file dyna the following routines are used:

- tempload, to calculate the instantaneous loading
- rhs, to determine the external force vector of the system
- results, to calculate all displacements, stresses and/or any other variables selected by the user

Notice that if nonzero boundary conditions are prescribed (base loading, e.g for earthquake calculations) the stiffness matrix of the system is used to calculate the steady state response to these nonzero conditions. It serves as particular solution in the modal dynamic solution procedure.

9.6.6 Steady state dynamics calculations

For steady state dynamics calculations the steady state response of the system to a harmonic excitation is again assumed to be a linear combination of the lowest eigenmodes. To this end, the eigenvalues and eigenmodes must have been calculated, either in the same run, or in a previous run. At the end of a frequency calculation this data, including the stiffness and mass matrix, is stored in binary form in a .eig file, provided the STORAGE=YES option is activated on the *FREQUENCY or *HEAT TRANSFER,FREQUENCY card. This file is read at the beginning of file steadystate.c.

In file steadystate.c the response is calculated in an explicit way, for details the reader is referred to [18]. Modal damping is allowed in the form of Rayleigh damping. Within file steadystate the following routines are used:

- tempload, to calculate the instantaneous loading
- rhs, to determine the external force vector of the system
- results, to calculate all displacements, stresses and/or any other variables selected by the user

Notice that if nonzero boundary conditions are prescribed (base loading, e.g for earthquake calculations) the stiffness matrix of the system is used to calculate the steady state response to these nonzero conditions. It serves as particular solution in the modal dynamic solution procedure.

9.7 Major routines

9.7.1 mafillsm

In this routine the different matrices are constructed. What has to be set up is summarized in the logicals mass, stiffness, buckling, rhsi and stiffonly. For instance, if the mass matrix must be calculated, mass=true, else mass=false. Notice that mass and stiffonly are defined as vectors of length 2. The first entry applies to mechanical calculations, the second entry to thermal calculations. If mass(1)=true the mass matrix for mechanical calculations or the mechanical part of coupled temperature-displacement calculations is determined and similarly, if mass(2)=true the specific heat matrix for thermal calculations or the thermal part of coupled temperature-displacement calculations is determined. This distinction is necessary to account for differences between mechanical and thermal calculations. It suffices to calculate the mass matrix in mechanical calculations only once, whereas the outspoken dependence of the specific heat on temperature requires the calculation of the specific heat matrix in each iteration. In what follows the mechanical stiffness matrix and thermal conductivity matrix will be simply called the stiffness matrix, the mechanical mass matrix and thermal heat capacity matrix will be called the mass matrix.

The routine consists of two major loops over all elements. The first loop constructs the mechanical part of the matrices, if applicable, the second loop constructs the thermal part, if applicable. Each loop runs over all elements, thereby collecting the element stiffness matrix and/or mass matrix from routine e_c3d and e_c3d_th for mechanical and thermal calculations, respectively, and inserting them into the global stiffness matrix and/or mass matrix, taking into account any linear multiple point constraints. The right-hand side matrices are also constructed from the element right-hand sides and any point loading.

To compose the element stiffness matrices the material stiffness matrices $(d\boldsymbol{\sigma}/d\boldsymbol{\epsilon})$ in the integration points of the elements are needed. These are recovered from storage from the last call to subroutine results.f. For the mass matrices the density and/or specific heat in the integration points is needed. These quantities are obtained by interpolation in the appropriate temperature range. No other material data need to be interpolated.

9.7.2 results

In subroutine results.f the dependent quantities in the finite element calculation, such as the displacements, stress, the internal forces, the temperatures and the heat flux, are determined from the independent quantities, i.e. the solution vector of the equation system. There are several modes in which results.f can be called, depending on the value of the variable iout:

- iout=-1: the displacements and temperatures are assumed to be known and used to calculate strains, stresses...., no result output
- iout=0: the displacements and temperatures are calculated from the system solution and subsequently used to calculate strains, stresses..., no result output
- iout=1: the displacements and temperatures are calculated from the system solution and subsequently used to calculate strains, stresses..., result output is requested (.dat or .frd file)
- iout=2: the displacements and temperatures are assumed to be known and used to calculate strains, stresses...., result output is requested (.dat or .frd file)

Calculating the displacements and/or temperatures from the result vector only involves the use of the relationship between the location in the solution vector and the physical degrees of freedom in the nodes (field nactdof), together with SPC and MPC information.

To obtain derived quantities such as stresses and heat flux a loop over all element integration points is performed. This is first done for mechanical quantities, then for heat transfer quantities.

In the mechanical loop the strain is determined from the displacements. For linear geometric calculations this is the infinitesimal strain, else it is the Lagrangian strain tensor [18]. For certain materials (e.g. the user defined materials) the deformation gradient is also determined. Then, materialdata_me.f is called, where the material data are obtained for the integration point and actual temperature (such as Young's modulus, thermal strain etc.). A subsequent call to mechmodel.f determines the local material gradient ($d\boldsymbol{\sigma}/d\boldsymbol{\epsilon}$) and the stress. From this the internal forces can be calculated.

The heat transfer loop is very similar: after calculation of the thermal gradient, the material data are interpolated in materialdata_th.f, the heat flux and tangent conductivity matrix ($d\boldsymbol{q}/d\boldsymbol{\Delta\theta}$) are determined in thermmodel.f and the concentrated internal heat vector is calculated.

The tangent material matrices determined in mechmodel.f and thermmodel.f are stored for further use in the construction of the element stiffness matrices (cf. mafillsm.f). An overview of the subroutine structure to calculate the stress and tangent material matrices and any related quantities is shown in Figure 150.

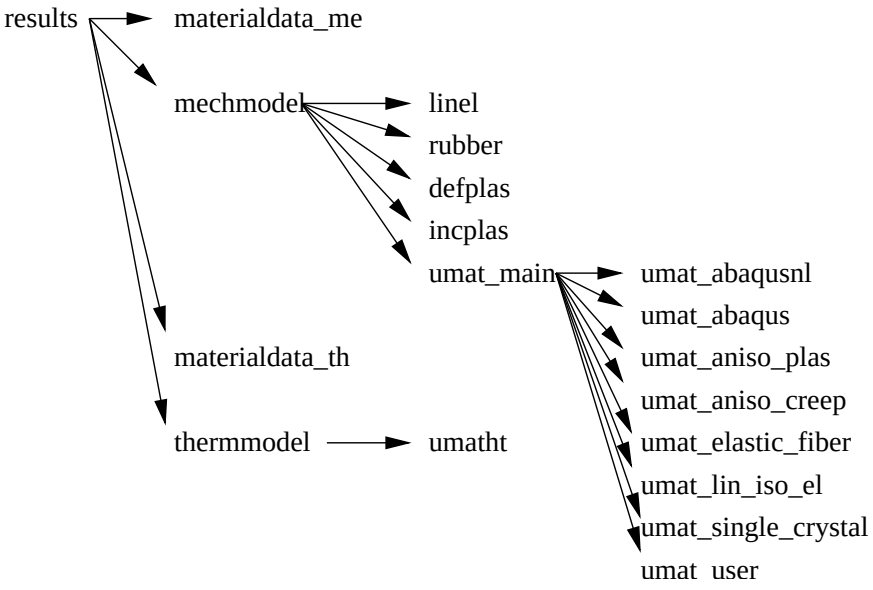


Figure 150: Flow diagram for subroutine results

Notice that the stresses and heat flux determined so far was calculated in the integration points. In the last part of results.f these values are extrapolated to the nodes, if requested by the user.

9.8 Aerodynamic and hydraulic networks

Aerodynamic and hydraulic networks are solved separately from the structural equation system. This is because networks generally lead to small sets of equations (at most a couple of thousand equations) which are inherently asymmetric. If solved together with the structural system, the small network contribution would lead to a complete asymmetric matrix and increase the computational time significantly. Moreover, especially aerodynamic networks are very nonlinear and require more iterations than structural nonlinearities. Consequently, the small network contribution would also lead to a lot more iterations. Therefore, the matrices of networks are set up and solved on their own taking the structural solution from the previous structural iteration as boundary condition. In a similar way, the network solution acts as boundary condition for the next structural iteration.

9.8.1 The variables and the equations

In Sections 6.9.16 and 6.9.17 the governing equations for aerodynamic and hydraulic networks were derived. It was shown that the basic variables for aerodynamic networks are the total temperature, the total pressure and the mass flow.

Table 20: Variables in fluid nodes.

DOF	corner node	midside node
0	total temperature	-
1	-	mass flow
2	total pressure	-
3	static temperature	geometry

In addition, one geometric parameter may be defined per element as additional unknown. This option has to be coded in the program in order to be active. Right now, this option only exists for the gate valve. All other variables can be calculated based on these three quantities. This is actually not a unique choice but seems to be best suited for our purposes. For hydraulic networks these reduce to the pressure, temperature and mass flow. This is completely different from the structural unknowns, which are taken to be the temperature and the displacements. Therefore, the degrees of freedom 0 to 3 which are used for structural calculations are redefined for networks according to Table (20)

A distinction is being made between corner nodes and midside nodes of fluid elements. Remember that network elements consist of two corner nodes and one middle node (Section 6.2.28). The mass flow is not necessarily uniquely determined at the corner nodes, since more than two branches can come together. Therefore, it is logical to define the mass flow as unknown in the middle of a network element. The same applies to the geometric parameter, if applicable. Similarly, the total temperature or total pressure may not be known within the element, since the exact location of discontinuities (such as enlargements or orifices) is not necessarily known. Consequently, it is advantageous to define the total temperature and total pressure as unknowns in the corner nodes. The static temperature is not a basic variable. Once the total temperature, mass flow and total pressure are known, the static temperature can be calculated. It is a derived quantity.

Similar to field nactdof for structural applications a field nactdog is introduced for network applications. It can be viewed as a matrix with 4 rows and as many columns as there are nodes in the model (including structural nodes; this is done to avoid additional pointing work between the local gas node number and the global node number). It indicates whether a specific degree of freedom in a gas node is active: if the entry is nonzero it is active, else it is inactive (which means that the value is known or not applicable because the node is a structural node). The degrees of freedom correspond to the first three rows of Table 20 and are repeated in Table 21 for clarity. Here too, only the first three rows are relevant.

Consequently, if nactdof(2,328) is nonzero, it means that the total pressure in node 328 is an unknown in the system. Actually, the nonzero value represents the number of the degree of freedom attached to the total pressure in node 328. The number of the degree of freedom corresponds with the column number

Table 21: Degrees of freedom in fluid nodes (field nactdog).

DOF	corner node	midside node
0	total temperature	-
1	-	mass flow
2	total pressure	-
3	-	geometry

Table 22: Conservation equations in fluid nodes (field nacteq).

DOF	corner node	midside node
0	energy	-
1	mass	-
2	-	momentum
3	if > 0: independent node of isothermal element the node belongs to;	-

in the resulting set of equations. What nactdof is for the degrees of freedom is nacteq for the equations. It is a field of the same size of nactdof but now a nonzero entry indicates that a specific conservation equation applies to the node, cf. Table 22.

If nacteq(1,8002) is nonzero, it means that the conservation of mass equation has to be formulated for node 8002. The nonzero value is actually the row number of this equation in the set of equations. If the value is zero, the equation does not apply, e.g. because the mass flow in all adjacent elements is known. The last row in field nacteq (at least for corner nodes) is used to account for isothermal conditions. These only apply to gas pipes of type GAS PIPE ISOTHERMAL and exit restrictors preceded by an isothermal gas pipe element. An isothermal element introduces an extra equation specifying that the static temperature in the two corner nodes of the pipe is equal. This can be transformed into a nonlinear equation in which the total temperature in one node (the dependent node) is written as a function of the total temperature in the other node and the other variables (total pressure in the nodes, mass flow). To account for this extra equation, the conservation of energy is not expressed for the dependent node (indeed, one can argue that, in order for the static temperatures to be equal an unknown amount of heat has to be introduced in the dependent node. So if nacteq(3,8002)=n is nonzero it means that node 8002 is the dependent node in an isothermal relation linking the static nodal temperature to the one of node n.

Field ineighe(i),i=1,...,ntg is used to determine the static temperature in an end node. If it is zero, node i is a mid-node. If it is equal to -1, the node is a chamber, for which the static temperature equals the total temperature. If it is

positive, its value is the element number of a gas pipe element or restrictor element, but not equal to a restrictor wall orifice, for which the static temperature is different from the total temperature. The mass flow of the referred element is used to calculate the static temperature from the total temperature.

9.8.2 Determining the basic characteristics of the network

In subroutine envtemp.f the basic properties of the network are determined. It is called at the start of nonlingeo.c. At first the gas nodes are identified and sorted. A node is a gas node if any of the following conditions is satisfied:

- it is used as environment node of a forced convection *FILM boundary condition. The temperature in such a node is an unknown. This also implies that a midside node of a network element cannot be used as environment node in a *FILM condition.

- it is used as environment node of a forced convection *DLOAD boundary condition. The total pressure in such a node is unknown (the static pressure may be more applicable for gas networks, this has not been implemented yet).

- it belongs to a network element. If it is an corner node the total temperature and the total pressure are unknowns, if it is a midside node the mass flow is unknown and the geometry may be unknown too.

In that way also the field nactdog is filled (with the value 1 for an unknown variable, 0 else). Next, the known boundary values (*BOUNDARY cards) are subtracted, and the unknown DOFs are numbered consecutively yielding the final form for nactdog. Notice that the global number of gas node i is itg(i). Since field its is ordered in an ascending order, subroutine nident.f can be used to find the local gas node number for a given global number. In the remaining test "gas node i" refers to the local number whereas "node i" refers to a global number.

In a loop over all network elements the necessary equations are determined. In a given corner node the conservation of mass equation is formulated if the mass flow in at least one of the adjacent network elements is unknown. The conservation of energy is written if the temperature in the corner node is unknown. Finally, conservation of momentum equation (also called element equation) is formulated for a midside node of a network element if not all quantities in the element equation are known. This latter check is performed in the subroutine flux.f (characterized by iflag=0). It contains on its own subroutines for several fluid section types, e.g. subroutine orifice.f for the fluid section of type ORIFICE. The number of unknowns relevant for the network element depends on its section type. After having identified all necessary equations in field nacteq they are numbered and the number of equations is compared with the number of unknowns. They must be equal in order to have a unique solution.

Next, multiple point constraints among network nodes are taken into account. They are defined using the *EQUATION keyword card. It is not allowed to use network nodes and non-network nodes in one and the same equation.

Finally, dependent and independent nodes are determined for each isothermal element and the appropriate entries in field nacteq (third row, cf. previous section) are defined. If at the stage of the matrix filling an corner node is a dependent node of an isothermal element the conservation of energy equation in that node is replaced by an equation that the static temperature in the dependent and independent node are equal. Fields ipogn and ign are deleted after leaving envtemp.f

9.8.3 Initializing the unknowns

Solving the structural system and the network is done in an alternating way. At the start of a network loop the unknowns (mass flow, total temperature, total pressure) are initialized. This is especially important for gas networks, since the initial values are taken as starting solution. Since the gas equations are very nonlinear, a good initial guess may accelerate the Newton-Raphson convergence quite a bit (or make a convergence possible in the first place).

At first an initial pressure distribution is determined. To that end the pressure value for nodes with a pressure boundary condition is stored in v (2,i), where i is the global node number. If no pressure boundary conditions applies, the minus the number of elements to which the node belongs is stored in the same field. If a node belongs to only one element, it is a boundary node and a fictitious initial pressure slightly smaller than the minimum pressure boundary condition is assigned to it. In that way, all boundary nodes are guaranteed to have a value assigned. The initial pressure in all other nodes is determined by solving for the Laplace equation in the network, i.e. the value in a node is the mean of the values in all surrounding nodes. To obtain a more realistic distribution the values are biased by an inverse tangent function, i.e. the values upstream decrease more slowly than on the downstream side of the network.

Another item taken care of at the start of initialnet.f is the determination of the number of gas pipe or restrictor elements the nodes belong to. If an end node i belongs to at most 2 elements of type gas pipe or restrictor and to no other elements one of the global element numbers is stored in ineighe(i) and the static temperature is determined from the other variables using the mass flow in this element. If not, the node is considered to be a big chamber for which total and static values coincide.

The temperature initial conditions are fixed at 293 K (only for those nodes for which no temperature boundary condition applies). In general, the temperature initial conditions are not so critical for the global convergence. For geometric quantities the initial value is zero. For the gate valve this is changed to the minimum allowable value of 0.125 (cf. liquidpipe.f).

Based on the total temperature and total pressure the mass flow in the elements is determined using the element equations. This is the second task to be accomplished by the element routines (characterized by iflag=1).

Finally, the static temperature is calculated for the nodes not identified as chambers based on the total pressure, total temperature and mass flow.

9.8.4 Calculating the residual and setting up the equation system

The residual of the governing equations is calculated in subroutine resultnet.f. At the start of the routine the static temperature is calculated for the nodes not identified as chambers based on the total pressure, total temperature and mass flow. Then, a loop is initialized covering all network elements. For each element the contributions to the conservation of mass equation and to the conservation of energy equation (or, equivalently, to the isothermal equation if the element is an isothermal gas pipe element) of its corner nodes are determined. Subsequently, the satisfaction of the element equation is verified. This is the third mode the element routines are called in, characterized by iflag=2. Finally, the energy contributions resulting from the interaction with the walls and due to prescribed heat generation in the network are taken into account. The residual constitutes the right hand side of the network system.

Setting up the equation system is done in subroutine mafillnet.f. The structure of the routine is very similar to the resultnet routine: in a loop over all elements the coefficients of the equations (conservation of mass and momentum and the conservation of energy, or, if applicable, the isothermal condition) are determined. This includes effects from the interaction with the walls. This leads to the left hand side of the system of equations.

9.8.5 Convergence criteria

Convergence is checked for the total temperature, mass flow, total pressure and geometry separately. Convergence is reaches if the change in solution in the last iteration does not exceed $10^{-4}x5x10^{-3}$ of the largest change in this network calculation or 10^{-8} times the largest absolute value within the network (cf. checkconvnet.c).

9.9 Three-Dimensional Navier-Stokes Calculations

Note: compressible CFD-calculations have been deactivated in version 2.7 due to unsatisfactory results. A new approach is being pursued.

9.10 List of variables and their meaning

Table 23: Variables in CalculiX.

variable	meaning
REARRANGEMENT OF THE ORDER IN THE INPUT DECK	
ifreeinp	next blank line in field inp
ipoinp(1,i)	index of the first column in field inp containing information on a block of lines in the input deck corresponding to fundamental key i; a fundamental key is a key for which the order in the input file matters (the fundamental keys are listed in file keystart.f)
ipoinp(2,i)	index of the last column in field inp containing information on a block of lines in the input deck corresponding to fundamental key i;
inp	a column i in field inp (i.e. inp(1..3,i)) corresponds to a uninterrupted block of lines assigned to one and the same fundamental key in the input deck. inp(1,i) is its first line in the input deck, inp(2,i) its last line and inp(3,i) the next column in inp corresponding to the same fundamental key; it takes the value 0 if none other exists.
MATERIAL DESCRIPTION	
nmat	# materials
matname(i)	name of material i
nelcon(1,i)	# (hyper)elastic constants for material i (negative kode for nonlinear elastic constants)
nelcon(2,i)	# temperature data points for the elastic constants of material i
elcon(0,j,i)	temperature at (hyper)elastic temperature point j of material i
elcon(k,j,i)	(hyper)elastic constant k at elastic temperature point j of material i
nrhcon(i)	# temperature data points for the density of material i
rhcon(0,j,i)	temperature at density temperature point j of material i
rhcon(1,j,i)	density at the density temperature point j of material i
nshcon(i)	# temperature data points for the specific heat of material i
shcon(0,j,i)	temperature at temperature point j of material i
shcon(1,j,i)	specific heat at constant pressure at the temperature point j of material i
shcon(2,j,i)	dynamic viscosity at the temperature point j of material i
shcon(3,1,i)	specific gas constant of material i
nalcon(1,i)	# of expansion constants for material i
nalcon(2,i)	# of temperature data points for the expansion coefficients of material i
alcon(0,j,i)	temperature at expansion temperature point j of material i

Table 23: (continued)

variable	meaning
alcon(k,j,i)	expansion coefficient k at expansion temperature point j of material i
ncocon(1,i)	# of conductivity constants for material i
ncocon(2,i)	# of temperature data points for the conductivity coefficients of material i
cocon(0,j,i)	temperature at conductivity temperature point j of material i
cocon(k,j,i)	conductivity coefficient k at conductivity temperature point j of material i
orname(i)	name of orientation i
orab(1..6,i)	coordinates of points a and b defining the new orientation
norien	# orientations
isotropic hardening	
nplicon(0,i)	# temperature data points for the isotropic hardening curve of material i
nplicon(j,i)	# of stress - plastic strain data points at temperature j for material i
plicon(0,j,i)	temperature data point j of material i
plicon(2*k-1,j,i)	stress corresponding to stress-plastic strain data point k at temperature data point j of material i
plicon(2*k-1,j,i)	for springs: force corresponding to force-displacement data point k at temperature data point j of material i
plicon(2*k-1,j,i)	for penalty contact: pressure corresponding to pressure-overclosure data point k at temperature data point j of material i
plicon(2*k,j,i)	plastic strain corresponding to stress-plastic strain data point k at temperature data point j of material i for springs: displacement corresponding to force-displacement data point k at temperature data point j of material i for penalty contact: overclosure corresponding to pressure-overclosure data point k at temperature data point j of material i
kinematic hardening	
nplkcon(0,i)	# temperature data points for the kinematic hardening curve of material i
nplkcon(j,i)	# of stress - plastic strain data points at temperature j for material i
plkcon(0,j,i)	temperature data point j of material i
plkcon(2*k-1,j,i)	stress corresponding to stress-plastic strain data point k at temperature data point j of material i

Table 23: (continued)

variable	meaning
	for penalty contact: conductance corresponding to conductance-pressure data point k at temperature data point j of material i
plkcon(2*k,j,i)	plastic strain corresponding to stress-plastic strain data point k at temperature data point j of material i
	for penalty contact: pressure corresponding to conductance-pressure data point k at temperature data point j of material i
kode=-1	Arrudy-Boyce
-2	Mooney-Rivlin
-3	Neo-Hooke
-4	Ogden (N=1)
-5	Ogden (N=2)
-6	Ogden (N=3)
-7	Polynomial (N=1)
-8	Polynomial (N=2)
-9	Polynomial (N=3)
-10	Reduced Polynomial (N=1)
-11	Reduced Polynomial (N=2)
-12	Reduced Polynomial (N=3)
-13	Van der Waals (not implemented yet)
-14	Yeoh
-15	Hyperfoam (N=1)
-16	Hyperfoam (N=2)
-17	Hyperfoam (N=3)
-50	deformation plasticity
-51	incremental plasticity (no viscosity)
-52	viscoplasticity
$<$ -100	user material routine with -kode-100 user defined constants with keyword *USER MATERIAL
PROCEDURE DESCRIPTION	
iperturb(1)	= 0 : linear
	= 1 : second order theory for frequency calculations following a static step (PERTURBATION selected)
	$\geq$ 2 : Newton-Raphson iterative procedure is active
	= 3 : nonlinear material (linear or nonlinear geometric and/or heat transfer)
iperturb(2)	0 : linear geometric (NLGEOM not selected)
	1 : nonlinear geometric (NLGEOM selected)
nmethod	1 : static (linear or nonlinear)
	2 : frequency(linear)
	3 : buckling (linear)
	4 : dynamic (linear or nonlinear)

Table 23: (continued)

variable	meaning
	5 : steady state dynamics
irstrt	0: no restart calculation
	-1: RESTART,READ; no RESTART,WRITE active
	n>0: frequency on a RESTART,WRITE card; RESTART, READ may be active
GEOMETRY DESCRIPTION	
nk	highest node number
co(i,j)	coordinate i of node j
inotr(1,j)	transformation number applicable in node j
inotr(2,j)	a SPC in a node j in which a transformation applies corresponds to a MPC. inotr(2,j) contains the number of a new node generated for the inhomogeneous part of the MPC
TOPOLOGY DESCRIPTION	
ne	highest element number
mi(1)	max # of integration points per element (max over all elements)
mi(2)	max degree of freedom per node (max over all nodes) in fields like v(0:mi(2))...
	if 0: only temperature DOF
	if 3: temperature + displacements
	if 4: temperature + displacements/velocities + pressure
kon(i)	field containing the connectivity lists of the elements in successive order
	for 1d and 2d elements (no composites) the 3d-expansion is stored first, followed by the topology of the original 1d or 2d element, for a shell composite this is followed by the topology of the expansion of each layer
For element i	
ipkon(i)	(location in kon of the first node in the element connectivity list of element i)-1
lakon(i)	element label
	C3D4: linear tetrahedral element (F3D4 for 3D-fluids)
	C3D6: linear wedge element (F3D6 for 3D-fluids)
	C3D6 E: expanded plane strain 3-node element = CPE3
	C3D6 S: expanded plane stress 3-node element = CPS3
	C3D6 A: expanded axisymmetric 3-node element = CAX3
	C3D6 L: expanded 3-node shell element = S3
	C3D8: linear hexahedral element (F3D8 for 3D-fluids)
	C3D8I: linear hexahedral element with incompatible modes
	C3D8I E: expanded plane strain 4-node element = CPE4
	C3D8I S: expanded plane stress 4-node element = CPS4
	C3D8I A: expanded axisymmetric 4-node element = CAX4

Table 23: (continued)

variable	meaning
	C3D8I L: expanded 4-node shell element = S4 C3D8I B: expanded 2-node beam element = B31 C3D8R: linear hexahedral element with reduced integration (F3D8R for 3D-fluids) C3D8R E: expanded plane strain 4-node element with reduced integration = CPE4R C3D8R S: expanded plane stress 4-node element with reduced integration = CPS4R C3D8R A: expanded axisymmetric 4-node element with reduced integration = CAX4R C3D8R L: expanded 4-node shell element with reduced integration = S4R C3D8R B: expanded 2-node beam element with reduced integration = B31R C3D10: quadratic tetrahedral element C3D15: quadratic wedge element C3D15 E: expanded plane strain 6-node element = CPE6 C3D15 S: expanded plane stress 6-node element = CPS6 C3D15 A: expanded axisymmetric 6-node element = CAX6 C3D15 L: expanded 6-node shell element = S6 C3D20: quadratic hexahedral element C3D20 E: expanded plane strain 8-node element = CPE8 C3D20 S: expanded plane stress 8-node element = CPS8 C3D20 A: expanded axisymmetric 8-node element = CAX8 C3D20 L: expanded 8-node shell element = S8 C3D20 B: expanded 3-node beam element = B32 C3D20R: quadratic hexahedral element with reduced integration C3D20RE: expanded plane strain 8-node element with reduced integration = CPE8R C3D20RS: expanded plane stress 8-node element with reduced integration = CPS8R C3D20RA: expanded axisymmetric 8-node element with reduced integration = CAX8R C3D20RL: expanded 8-node shell element with reduced integration = S8R C3D20RLC: expanded composite 8-node shell element with reduced integration = S8R C3D20RB: expanded 3-node beam element with reduced integration = B32R GAPUNI: 2-node gap element ESPRNGA1 : 2-node spring element EDSHPTA1 : 2-node dashpot element

Table 23: (continued)

variable	meaning
	ESPRNGC3 : 4-node contact spring element ESPRNGC4 : 5-node contact spring element ESPRNGC6 : 7-node contact spring element ESPRNGC8 : 9-node contact spring element ESPRNGC9 : 10-node contact spring element ESPRNGF3 : 4-node advection spring element ESPRNGF4 : 5-node advection spring element ESPRNGF6 : 7-node advection spring element ESPRNGF8 : 9-node advection spring element **network elements (D-type):**] DATR : absolute to relative DCARBS : carbon seal DCARBSGE : carbon seal GE (proprietary) DCHAR : characteristic DGAPFA : gas pipe Fanno adiabatic DGAPFAA : gas pipe Fanno adiabatic Albers (proprietary) DGAPFAF : gas pipe Fanno adiabatic Friedel (proprietary) DGAPFI : gas pipe Fanno isothermal DGAPFIA : gas pipe Fanno isothermal Albers (proprietary) DGAPFIF : gas pipe Fanno isothermal Friedel (proprietary) DGAPIA : gas pipe adiabatic DGAPIAA : gas pipe adiabatic Albers (proprietary) DGAPIAF : gas pipe adiabatic Friedel (proprietary) DGAPII : gas pipe isothermal DGAPIIA : gas pipe isothermal Albers (proprietary) DGAPIIF : gas pipe isothermal Friedel (proprietary) DLABD : labyrinth dummy (proprietary) DLABFSN : labyrinth flexible single DLABFSP : labyrinth flexible stepped DLABFSR : labyrinth flexible straight DLABSN : labyrinth single DLABSP : labyrinth stepped DLABSR : labyrinth straight DLDOP : oil pump (proprietary) DLICH : channel straight DLICHCO : channel contraction DLICHDO : channel discontinuous opening DLICHDR : channel drop DLICHDS : channel discontinuous slope DLICHEL : channel enlargement DLICHRE : channel reservoir

Table 23: (continued)

variable	meaning
	DLICHSG : channel sluice gate DLICHSO : channel sluice opening DLICHST : channel step DLICHWE : channel weir crest DLICHWO : channel weir slope DLIPIBE : (liquid) pipe bend DLIPIBR : (liquid) pipe branch (not available yet) DLIPICO : (liquid) pipe contraction DLIPIDI : (liquid) pipe diaphragm DLIPIEL : (liquid) pipe enlargement DLIPIEN : (liquid) pipe entrance DLIPIGV : (liquid) pipe gate valve DLIPIMA : (liquid) pipe Manning DLIPIMAF : (liquid) pipe Manning flexible DLIPIWC : (liquid) pipe White-Colebrook DLIPIWCF : (liquid) pipe White-Colebrook flexible DLIPU : liquid pump DLPBEIDC : (liquid) restrictor bend Idelchik circular DLPBEIDR : (liquid) restrictor bend Idelchik rectangular DLPBEMA : (liquid) restrictor own (proprietary) DLPBEMI : (liquid) restrictor bend Miller DLPBRJG : branch joint GE DLPBRJI1 : branch joint Idelchik1 DLPBRJI2 : branch joint Idelchik2 DLPBRSG : branch split GE DLPBRSI1 : branch split Idelchik1 DLPBRSI2 : branch split Idelchik2 DLPC1 : (liquid) orifice Cd=1 DLPCO : (liquid) restrictor contraction DLPEL : (liquid) restrictor enlargement DLPEN : (liquid) restrictor entry DLPEX : (liquid) restrictor exit DLPLOID : (liquid) restrictor long orifice Idelchik DLPLOLI : (liquid) restrictor long orifice Lichtarowicz DLPUS : (liquid) restrictor user DLPVF : (liquid) vortex free DLPVS : (liquid) vortex forced DLPWAOR : (liquid) restrictor wall orifice DMRGF : Moehring centrifugal DMRGP : Moehring centripetal DORBG : orifice Bragg (proprietary) DORBT : bleed tapping DORC1 : orifice Cd=1

Table 23: (continued)

variable	meaning
	DORMA : orifice proprietary, rotational correction Albers (proprietary) DORMM : orifice McGreehan Schotsch, rotational correction McGreehan and Schotsch DORPA : orifice Parker and Kercher, rotational correction Albers (proprietary) DORPM : orifice Parker and Kercher, rotational correction McGreehan and Schotsch DORPN : preswirl nozzle DREBEIDC : restrictor bend Idelchik circular DREBEIDR : restrictor bend Idelchik rectangular DREBEMA : restrictor own (proprietary) DREBEMI : restrictor bend Miller DREBRJG : branch joint GE DREBRJI1 : branch joint Idelchik1 DREBRJI2 : branch joint Idelchik2 DREBRSG : branch split GE DREBRSI1 : branch split Idelchik1 DREBRSI2 : branch split Idelchik2 DRECO : restrictor contraction DREEL : restrictor enlargement DREEN : restrictor entrance DREEX : restrictor exit DRELOID : restrictor long orifice Idelchik DRELOLI : restrictor long orifice Lichtarowicz DREUS : restrictor user DREWAOR : restrictor wall orifice DRIMS : rim seal (proprietary) DRTA : relative to absolute DSPUMP : scavenge pump (proprietary) DVOFO : vortex forced DVOFR : vortex free
ielorien(j,i)	orientation number of layer j
ielmat(j,i)	material number of layer j
ielprop(i)	property number (for gas networks)
SETS AND SURFACES	
nset	number of sets (including surfaces)
ialset(i)	member of a set or surface: this is a - node for a node set or nodal surface - element for an element set - number made up of 10*(element number)+facial number for an element face surface

Table 23: (continued)

variable	meaning
	if ialset(i)=-1 it means that all nodes or elements (depending on the kind of set) in between ialset(i-2) and ialset(i-1) are also member of the set
For set i	
set(i)	name of the set; this is the user defined name + N for node sets + E for element sets + S for nodal surfaces + T for element face surfaces
istartset(i)	pointer into ialset containing the first set member
iendset(i)	pointer into ialset containing the last set member
TIE CONSTRAINTS	
ntie	number of tie constraints
For tie constraint i	
tieset(1,i)	name of the tie constraint; for contact constraints (which do not have a name) the adjust nodal set name is stored, if any, and a C is appended at the end for multistage constraints a M is appended at the end for a contact tie a T is appended at the end for submodels (which do not have a name) a fictitious name SUBMODELi is used, where i is a three-digit consecutive number and a S is appended at the end
tieset(2,i)	dependent surface name + S
tieset(3,i)	independent surface name + S for nodal surfaces + T for element face surfaces
tietol(1,i)	tie tolerance; used for cyclic symmetry ties special meaning for contact pairs: > 0 for large sliding < 0 for small sliding if $\|\text{tietol}\| \geq 2$, adjust value = $\|\text{tietol}\|$-2
tietol(2,i)	only for contact pairs: number of the relevant interaction definition (is treated as a material)
CONTACT	
ncont	total number of triangles in the triangulation of all independent surfaces
ncone	total number of slave nodes in the contact formulation
For triangle i	
koncont(1..3,i)	nodes belonging to the triangle
koncont(4,i)	element face to which the triangle belongs: 10*(element number) + face number

Table 23: (continued)

variable	meaning
cg(1..3,i)	global coordinates of the center of gravity
straight(1..4,i)	coefficients of the equation of the plane perpendicular to the triangle and containing its first edge (going through the first and second node of koncont)
straight(5..8,i)	idem for the second edge
straight(9..12,i)	idem for the third edge
straight(13..16,i)	coefficients of the equation of the plane containing the triangle
For contact tie constraint i	
itietri(1,i)	first triangle in field koncont of the master surface corresponding to contact tie constraint i
itietri(2,i)	last triangle in field koncont of the master surface corresponding to contact tie constraint i
SHELL (2D) AND BEAM (1D) VARIABLES (INCLUDING PLANE STRAIN, PLANE STRESS AND AXISYMMETRIC ELEMENTS)	
iponor(2,i)	two pointers for entry i of kon. The first pointer points to the location in xnor preceding the normals of entry i, the second points to the location in knor of the newly generated dependent nodes of entry i.
xnor(i)	field containing the normals in nodes on the elements they belong to
knor(i)	field containing the extra nodes needed to expand the shell and beam elements to volume elements
thickn(2,i)	thicknesses (one for shells, two for beams) in node i
thicke(j,i)	thicknesses (one (j=1) for non-composite shells, two (j=1,2) for beams and n (j=1..n) for composite shells consisting of n layers) in element nodes. The entries correspond to the nodal entries in field kon
offset(2,i)	offsets (one for shells, two for beams) in element i
iponoel(i)	pointer for node i into field inoel, which stores the 1D and 2D elements belonging to the node.
inoel(3,i)	field containing an element number, a local node number within this element and a pointer to another entry (or zero if there is no other).
inoelfree	next free field in inoel

Table 23: (continued)

variable	meaning
rig(i)	integer field indicating whether node i is a rigid node (nonzero value) or not (zero value). In a rigid node or knot all expansion nodes except the ones not in the midface of plane stress, plane strain and axisymmetric elements are connected with a rigid body MPC. If node i is a rigid node rig(i) is the number of the rotational node of the knot; if the node belongs to axisymmetric, plane stress and plane strain elements only, no rotational node is linked to the knot and rig(i)=-1
AMPLITUDES	
nam	# amplitude definitions
amta(1,j)	time of (time,amplitude) pair j
amta(2,j)	amplitude of (time,amplitude) pair j
namtot	total # of (time,amplitude) pairs
For amplitude i	
amname(i)	name of the amplitude
namta(1,i)	location of first (time,amplitude) pair in field amta
namta(2,i)	location of last (time,amplitude) pair in field amta
namta(3,i)	in absolute value the amplitude it refers to; if abs(namta(3,i))=i it refers to itself. If abs(namta(3,i))=j, amplitude i is a time delay of amplitude j the value of which is stored in amta(1,namta(1,i)); in the latter case amta(2,namta(1,i)) is without meaning; If namta(3,i)>0 the time in amta for amplitude i is step time, else it is total time.
TRANSFORMS	
ntrans	# transform definitions
trab(1..6,i)	coordinates of two points defining the transform
trab(7,i)	=-1 for cylindrical transformations =1 for rectangular transformations
SINGLE POINT CONSTRAINTS	
nboun	# SPC's
For SPC i	
nodeboun(i)	SPC node
ndirboun(i)	SPC direction
typeboun(i)	SPC type (SPCs can contain the nonhomogeneous part of MPCs) B=prescribed boundary condition M=midplane P=planempc R=rigidbody S=straightmpc

Table 23: (continued)

variable	meaning
	U=usermpc
	L=submodel
xboun(i)	magnitude of constraint at end of a step
xbounold(i)	magnitude of constraint at beginning of a step
xbounact(i)	magnitude of constraint at the end of the present increment
xbounini(i)	magnitude of constraint at the start of the present increment
iamboun(i)	amplitude number
	for submodels the step number is inserted
ikboun(i)	ordered array of the DOFs corresponding to the SPC's (DOF=8*(nodeboun(i)-1)+ndirboun(i))
ilboun(i)	original SPC number for ikboun(i)
MULTIPLE POINT CONSTRAINTS	
j=ipompc(i)	starting location in nodempc and coefmpc of MPC i
nodempc(1,j)	node of first term of MPC i
nodempc(2,j)	direction of first term of MPC i
k=nodempc(3,j)	next entry in field nodempc for MPC i (if zero: no more terms in MPC)
coefmpc(j)	first coefficient belonging to MPC i
nodempc(1,k)	node of second term of MPC i
nodempc(2,k)	direction of second term of MPC i
coefmpc(k)	coefficient of second term of MPC i
ikmpc (i)	ordered array of the dependent DOFs corresponding to the MPC's DOF=8*(nodempc(1,ipompc(i))-1)+nodempc(2,ipompc(i))
ilmpc (i)	original MPC number for ikmpc(i)
icascade	0 : MPC's did not change since the last iteration
	1 : MPC's changed since last iteration : dependency check in cascade.c necessary
	2 : at least one nonlinear MPC had DOFs in common with a linear MPC or another nonlinear MPC. dependency check is necessary in each iteration
POINT LOADS	
nforc	# of point loads
For point load i	
nodeforc(1,i)	node in which force is applied
nodeforc(2,i)	sector number, if force is real; sector number + # sectors if force is imaginary (only for modal dynamics and steady state dynamics analyses with cyclic symmetry)
ndirforc(i)	direction of force
xforc(i)	magnitude of force at end of a step
xforcold(i)	magnitude of force at start of a step

Table 23: (continued)

variable	meaning
xforcact(i)	actual magnitude
iamforc(i)	amplitude number
ikforc(i)	ordered array of the DOFs corresponding to the point loads (DOF=8*(nodeboun(i)-1)+ndirboun(i))
ilforc(i)	original SPC number for ikforc(i)
FACIAL DISTRIBUTED LOADS	
nload	# of facial distributed loads
For distributed load i	
nelemload(1,i)	element to which distributed load is applied
nelemload(2,i)	node for the environment temperature (only for heat transfer analyses); sector number, if load is real; sector number + # sectors if load is imaginary (only for modal dynamics and steady state dynamics analyses with cyclic symmetry)
sideload(i)	load label; indicated element side to which load is applied
xload(1,i)	magnitude of load at end of a step or, for heat transfer analyses, the convection (*FILM) or the radiation coefficient (*RADIATE)
xload(2,i)	the environment temperature (only for heat transfer analyses
xloadold(1..2,i)	magnitude of load at start of a step
xloadact(1..2,i)	actual magnitude of load
iamload(1,i)	amplitude number for xload(1,i) for submodels the step number is inserted
iamload(2,i)	amplitude number for xload(2,i)
MASS FLOW RATE	
nflow	# of network elements
TEMPERATURE LOADS	
t0(i)	initial temperature in node i at the start of the calculation
t1(i)	temperature at the end of a step in node i
t1old(i)	temperature at the start of a step in node i
t1act(i)	actual temperature in node i
iamt1(i)	amplitude number
MECHANICAL BODY LOADS	
nbody	# of mechanical body loads
For body load i	
ibody(1,i)	code identifying the kind of body load 1: centrifugal loading 2: gravity loading with known gravity vector 3: generalized gravity loading
ibody(2,i)	amplitude number for load i
ibody(3,i)	load case number for load i

Table 23: (continued)

variable	meaning
cbody(i)	element number or element set to which load i applies
xbody(1,i)	size of the body load
xbody(2..4,i)	for centrifugal loading: point on the axis for gravity loading with known gravity vector: normalized gravity vector
xbody(5..7,i)	for centrifugal loading: normalized vector on the rotation axis
xbodyact(1,i)	actual magnitude of load
xbodyact(2..7,i)	identical to the corresponding entries in xbody
For element i	
ipobody(1,i)	body load applied to element i, if any, else 0
ipobody(2,i)	index referring to the line in field ipobody containing the next body load applied to element i, i.e. ipobody(1,ipobody(2,i)), else 0
STRESS, STRAIN AND ENERGY FIELDS	
eei(i,j,k)	in general : Lagrange strain component i in integration point j of element k (linear strain in linear elastic calculations) for elements with DEFORMATION PLASTICITY property: Eulerian strain component i in integration point j of element k (linear strain in linear elastic calculations)
eeiini(i,j,k)	Lagrange strain component i in integration point of element k at the start of an increment
een(i,j)	Lagrange strain component i in node j (mean over all adjacent elements linear strain in linear elastic calculations)
stx(i,j,k)	Cauchy or PK2 stress component i in integration point j of element k at the end of an iteration (linear stress in linear elastic calculations). For spring elements stx(1..3,1,k) contains the relative displacements for element k and stx(4..6,1,k) the contact stresses
sti(i,j,k)	PK2 stress component i in integration point j of element k at the start of an iteration (linear stress in linear elastic calculations)
stiini(i,j,k)	PK2 stress component i in integration point j of element k at the start of an increment
stn(i,j)	Cauchy stress component i in node j (mean over all adjacent elements; "linear" stress in linear elastic calculations)
ener(j,k)	strain energy in integration point j of element k
ener(j,ne+k)	kinetic energy in integration point j of element k (only for *EL PRINT)
enerini(j,k)	strain energy in integration point of element k at the start of an increment

Table 23: (continued)

variable	meaning
enern(j)	strain energy in node j (mean over all adjacent elements
THERMAL ANALYSIS	
ithermal(1) (in this manual also called ithermal)	0 : no temperatures involved in the calculation 1 : stress analysis with given temperature field 2 : thermal analysis (no displacements) 3 : coupled thermal-mechanical analysis : temperatures and displacements are solved for simultaneously
ithermal(2)	used to determine boundary conditions for plane stress, plane strain and axisymmetric elements 0 : no temperatures involved in the calculation 1 : no heat transfer nor coupled steps in the input deck 2 : no mechanical nor coupled steps in the input deck 3 : at least one mechanical and one thermal step or at least one coupled step in the input deck
v(0,j)	temperature of node j at the end of an iteration (for ithermal > 1)
vold(0,j)	temperature of node j at the start of an iteration (for ithermal > 1)
vini(0,j)	temperature of node j at the start of an increment (for ithermal > 1)
fn(0,j)	actual temperature at node j (for ithermal > 1)
qfx(i,j,k)	heat flux component i in integration point j of element k at the end of an iteration
qfn(i,j)	heat flux component i in node j (mean over all adjacent elements)
DISPLACEMENTS AND SPATIAL/TIME DERIVATIVES	
v(i,j)	displacement of node j in direction i at the end of an iteration
vold(i,j)	displacement of node j in direction i at the start of an iteration
vini(i,j)	displacement of node j in direction i at the start of an increment
ve(i,j)	velocity of node j in direction i at the end of an iteration
veold(i,j)	velocity of node j in direction i at the start of an iteration
veini(i,j)	velocity of node j in direction i at the start of an increment
accold(i,j)	acceleration of node j in direction i at the start of an iteration
accini(i,j)	acceleration of node j in direction i at the start of an increment
vkl(i,j)	(i,j) component of the displacement gradient tensor at the end of an iteration
xkl(i,j)	(i,j) component of the deformation gradient tensor at the end of an iteration

Table 23: (continued)

variable	meaning
xikl(i,j)	(i,j) component of the deformation gradient tensor at the start of an increment
ckl(i,j)	(i,j) component of the inverse of the deformation gradient tensor
LINEAR EQUATION SYSTEM	
nasym	0: symmetrical system 1: asymmetrical system
ad(i)	element i on diagonal of stiffness matrix
au(i)	element i in upper triangle of stiffness matrix
irow(i)	row of element i in field au (i.e. au(i))
icol(i)	number of subdiagonal nonzero's in column i (only for symmetric matrices)
jq(i)	location in field irow of the first subdiagonal nonzero in column i (only for symmetric matrices)
adb(i)	element i on diagonal of mass matrix, or, for buckling, of the incremental stiffness matrix (only nonzero elements are stored)
aub(i)	element i in upper triangle of mass matrix, or, for buckling, of the incremental stiffness matrix (only nonzero elements are stored)
neq[0]	# of mechanical equations
neq[1]	sum of mechanical and thermal equations
neq[2]	neq[1] + # of single point constraints (only for modal calculations)
nzl	number of the column such that all columns with a higher column number do not contain any (projected) nonzero off-diagonal terms ($\leq$ neq[1])
nzs[0]	sum of projected nonzero mechanical off-diagonal terms
nzs[1]	nzs[0]+sum of projected nonzero thermal off-diagonal terms
nzs[2]	nzs[1] + sum of nonzero coefficients of SPC degrees of freedom (only for modal calculations)
nactdof(i,j)	actual degree of freedom (in the system of equations) of DOF i of node j (0 if not active)
inputformat	=0: matrix is symmetric; lower triangular matrix is stored in fields ad (diagonal), au (subdiagonal elements), irow, icol and jq. =1: matrix is not symmetric. Diagonal and subdiagonal entries are stored as for inputformat=0; The superdiagonal entries are stored at the end of au in exactly the same order as the symmetric subdiagonal counterpart
INTERNAL AND EXTERNAL FORCES	

Table 23: (continued)

variable	meaning
fext(i)	external mechanical forces in DOF i (due to point loads and distributed loads, including centrifugal and gravity loads, but excluding temperature loading and displacement loading)
fextini(i)	external mechanical forces in DOF i (due to point loads and distributed loads, including centrifugal and gravity loads, but excluding temperature loading and displacement loading) at the end of the last increment
finc(i)	external mechanical forces in DOF i augmented by contributions due to temperature loading and prescribed displacements; used in linear calculations only
f(i)	actual internal forces in DOF i due to : actual displacements in the independent nodes; prescribed displacements at the end of the increment in the dependent nodes; temperatures at the end of the increment in all nodes
fini(i)	internal forces in DOF i at the end of the last increment
b(i)	right hand side of the equation system : difference between fext and f in nonlinear calcultions; for linear calculations, b=finc.
fn(i,j)	actual force at node j in direction i
INCREMENT PARAMETERS	
tinc	user given increment size (can be modified by the program if the parameter DIRECT is not activated)
tper	user given step size
dtheta	normalized (by tper) increment size
theta	normalized (by tper) size of all previous increments (not including the present increment)
reltime	theta+dtheta
dtime	real time increment size
time	real time size of all previous increments INCLUDING the present increment
ttime	real time size of all previous steps
DIRECT INTEGRATION DYNAMICS	
alpha,bet,gam	parameter in the alpha-method of Hilber, Hughes and Taylor
iexpl	=0 : implicit dynamics =1 : explicit dynamics
FREQUENCY CALCULATIONS	
mei[0]	number of requested eigenvalues
mei[1]	number of Lanczos vectors
mei[2]	maximum number of iterations

Table 23: (continued)

variable	meaning
mei[3]	if 1: store eigenfrequencies, eigenmodes, mass matrix and possibly stiffness matrix in .eig file, else 0
fei[0]	tolerance (accuracy)
fei[1]	lower value of requested frequency range
fei[2]	upper value of requested frequency range
CYCLIC SYMMETRY CALCULATIONS	
mcs	number of cyclic symmetry parts
ics	one-dimensional field; contains all independent nodes, one part after the other, and sorted within each part
rcs	one-dimensional field; contains the corresponding radial coordinates
zcs	one-dimensional field; contains the corresponding axial coordinates
For cyclic symmetry part i	
cs(1,i)	number of segments in 360°
cs(2,i)	minimum nodal diameter
cs(3,i)	maximum nodal diameter
cs(4,i)	number of nodes on the independent side
cs(5,i)	number of sections to be plotted
cs(6..12,i)	coordinates of two points on the cyclic symmetry axis
cs(13,i)	number of the element set (for plotting purposes)
cs(14,i)	total number of independent nodes in all previously defined cyclic symmetry parts
cs(15,i)	cos(angle) where angle = 2*π/cs(1,mcs)
cs(16,i)	sin(angle) where angle = 2*π/cs(1,mcs)
cs(17,i)	number of tie constraint
MODAL DYNAMICS AND STEADY STATE DYNAMICS CALCULATIONS	
	For Rayleigh damping (modal and steady state dynamics)
xmodal(1)	α_m (first Rayleigh coefficient)
xmodal(2)	β_m (second Rayleigh coefficient)
	For steady state dynamics
xmodal(3)	lower frequency bound f_{min}
xmodal(4)	upper frequency bound f_{max}
xmodal(5)	number of data points $n_{data} + 0.5$
xmodal(6)	bias
xmodal(7)	if harmonic: -0.5; if not harmonic: number of Fourier coefficients + 0.5
xmodal(8)	lower time bound t_{min} for one period (nonharmonic loading)
xmodal(9)	upper time bound t_{max} for one period (nonharmonic loading)

Table 23: (continued)

variable	meaning
	For damping (modal and steady state dynamics)
xmodal(10)	internal number of node set for which results are to be calculated
xmodal(11)	for Rayleigh damping: -0.5 for direct damping: largest mode for which ζ is defined +0.5
	For direct damping
xmodal(12.. int(xmodal(11)))	values of the ζ coefficients
OUTPUT IN .DAT FILE	
prset(i)	node or element set corresponding to output request i
prlab(i)	label corresponding to output request i. It contains 6 characters. The first 4 are reserved for the field name, e.g. 'U ' for displacements, the fifth for the value of the TOTALS parameter ('T' for TOTALS=YES, 'O' for TOTALS=ONLY and ' ' else) and the sixth for the value of the GLOBAL parameter ('G' for GLOBAL=YES and 'L' for GLOBAL=NO).
nprint	number of print requests

Table 23: (continued)

variable	meaning
OUTPUT IN .FRD FILE	
filab(i)	label corresponding to output field i. It contains 6 characters. The first 4 are reserved for the field name. The order is fixed: filab(1)='U ', filab(2)='NT ',filab(3)='S ',filab(4)='E ', filab(5)='RF ', filab(6)='PEEQ', filab(7)='ENER', filab(8)='SDV ', filab(9)='HFL ', filab(10)='RFL ', filab(11)='PU ', filab(12)='PNT ', filab(13)='ZZS ', filab(14)='TT ', filab(15)='MF ', filab(16)='PT ', filab(17)='TS ', filab(18)='PHS ', filab(19)='MAXU',filab(20)='MAXS', filab(21)='V ',filab(22)='PS ',filab(23)='MACH', filab(24)='CP ', filab(25)='TURB', filab(26)='CONT ' filab(27)='CELS ', filab(28)='DEPT ', filab(29)='HCRI ', filab(30)='MAXE', filab(31)='PRF ', filab(32)='ME ' and filab(33)='HER . Results are stored for the complete mesh. A field is not selected if the first 4 characters are blank, e.g. the stress is not stored if filab(3)(1:4)=' '. An exception to this rule is formed for filab(1): here, only the first two characters are used and should be either 'U ' or ' ', depending on whether displacements are requested are not. The third character takes the value 'C' if the user wishes that the contact elements in each iteration of the last increment are stored in dedicated files, else it is blank. The fourth character takes the value 'I' if the user wishes that the displacements of the iterations of the last increment are stored (used for debugging in case of divergence), else it is blank. If the mesh contains 1D or 2D elements, the fifth character takes the value 'I' if the results are to be interpolated, 'M' if the section forces are requested instead of the stresses and 'E' if the 1D/2D element results are to be given on the expanded elements. In all other cases the fifth character is blank: ' '. The sixth character contains the value of the GLOBAL parameter ('G' for GLOBAL=YES and 'L' for GLOBAL=NO). The entries filab(13)='RFRES ' and filab(14)='RFLRES' are reserved for the output of the residual forces and heat fluxes in case of no convergence and cannot be selected by the user: the residual forces and heat fluxes are automatically stored if the calculation stops due to divergence.
inum(i)	=-1: network node =1: structural node or 3D fluid node
CONVECTION NETWORKS	
ntg	number of gas nodes

Table 23: (continued)

variable	meaning
For gas node i	
itg(i)	global node number
nactdog(j,i)	if $\neq 0$ indicates that degree of freedom j of gas node i is is an unknown; the nonzero number is the column number of the DOF in the convection system of equations. The physical significance of j depends on whether the node is a midside node or corner node of a fluid element: j=0 and corner node: total temperature j=1 and midside node: mass flow j=2 and corner node: total pressure j=3 and midside node: geometry (e.g. α for a gate valve)
nacteq(j,i)	if $\neq 0$ indicates that equation type j is active in gas node i; the nonzero number is the row number of the DOF in the convection system of equations. The equation type of j depends on whether the node is a midside node or corner node of a network element: j=0 and corner node: conservation of energy j=1 and corner node: conservation of mass j=2 and midside node: convervation of momentum
ineighe(i)	only for gas network nodes (no liquids): if 0: itg(i) is a midside node if -1: itg(i) is a chamber if > 0: ineighe(i) is a gas pipe element itg(i) belongs to
v(j,i)	value of degree of freedom j in node i (global numbering). The physical significance of j depends on whether the node is a midside node or corner node of a network element: j=0 and corner node: total temperature j=1 and midside node: mass flow j=2 and corner node: total pressure j=3 and corner node: static temperature j=3 and midside node: geometry
nflow	number of network elements
ieg(i)	global element number corresponding to network element i
network	if 0: purely thermal (only unknowns: total temperature) if 1: coupled thermodynamic network if 2: purely aerodynamic (total temperature is known everywhere)
THERMAL RADIATION	
ntr	number of element faces loaded by radiation = radiation faces
iviewfile	< 0: reading the viewfactors from file

Table 23: (continued)

variable	meaning
	≥ 0: calculating the viewfactors
| iviewfile |	≥ 2: write the viewfactors to file < 2: do not write the viewfactors to file $= 3$: stop after storing the viewfactors to file
For radiation face i	
kontri(1..3,j)	nodes belonging to triangle j
kontri(4,j)	radiation face number (> 0 and $\leq$ ntri)to which triangle j belongs
nloadtr(i)	distributed load number (> 0 and $\leq$ nload) corresponding to radiation face i
ITERATION VARIABLES	
istep	step number
iinc	increment number
iit	iteration number = -1 only before the first iteration in the first increment of a step = 0 before the first iteration in an increment which was repeated due to non-convergence or any other but the first increment of a step > 0 denotes the actual iteration number
PHYSICAL CONSTANTS	
physcon(1)	Absolute zero
physcon(2)	Stefan-Boltzmann constant
physcon(3)	Newton Gravity constant
physcon(4)	Static temperature at infinity (for 3D fluids)
physcon(5)	Velocity at infinity (for 3D fluids)
physcon(6)	Static pressure at infinity (for 3D fluids)
physcon(7)	Density at infinity (for 3D fluids)
physcon(8)	Typical size of the computational domain (for 3D fluids)
physcon(9)	Perturbation parameter if $0 \leq physcon(9) < 1$: laminar if $1 \leq physcon(9) < 2$: k-ϵ Model if $2 \leq physcon(9) < 3$: q-ω Model if $3 \leq physcon(9) < 4$: SST Model
COMPUTATIONAL FLUID DYNAMICS	
vold(0,i)	Static temperature in node i
vold(1..3,i)	Velocity components in node i
vold(4,i)	Pressure in node i
voldaux(0,i)	Total energy density $\rho\epsilon_t$ in node i
voldaux(1..3,i)	Momentum density components ρv_i in node i

Table 23: (continued)

variable	meaning
voldaux(4,i)	Density ρ in node i
v(0,i)	Total energy density correction in node i
v(1..3,i)	Momentum density correction components in node i
v(4,i)	For fluids: Pressure correction in node i For gas: Density correction in node i
CONVERGENCE PARAMETERS	
qam[0]	$\tilde{q}_i^\alpha$ for the mechanical forces
qam[1]	$\tilde{q}_i^\alpha$ for the concentrated heat flux
ram[0]	$r_{i,max}^\alpha$ for the mechanical forces
ram[1]	$r_{i,max}^\alpha$ for the concentrated heat flux
ram[2]	the node corresponding to ram[0]
ram[3]	the node corresponding to ram[1]
uam[0]	$\Delta u_{i,max}^\alpha$ for the displacements
uam[1]	$\Delta u_{i,max}^\alpha$ for the temperatures
cam[0]	$c_{i,max}^\alpha$ for the displacements
cam[1]	$c_{i,max}^\alpha$ for the temperatures
cam[2]	largest temperature change within the increment
cam[3]	node corresponding to cam[0]
cam[4]	node corresponding to cam[1]
	for networks
uamt	largest increment of gas temperature
camt[0]	largest correction to gas temperature
camt[1]	node corresponding to camt[0]
uamf	largest increment of gas massflow
camf[0]	largest correction to gas massflow
camf[1]	node corresponding to camt[0]
uamp	largest increment of gas pressure
camp[0]	largest correction to gas pressure
camp[1]	node corresponding to camt[0]
THREE-DIMENSIONAL INTERPOLATION	
cotet(1..3,i)	coordinates of nodes i
kontet(1..4,i)	nodes belonging to tetrahedron i
ipofa(i)	entry in field inodfa pointing to a face for which node i is the smallest number
inodfa(1..3,i)	nodes j, k and l belonging to face i such that $j < k < l$
inodfa(4,i)	number of another face for which inodfa(1,i) is the smallest number. If no other exists the value is zero
planfa(1..4,i)	coefficients a, b, c and d of the plane equation ax+by+cz+d=0 of face i
ifatet(1..4,i)	faces belonging to tetrahedron i. The sign identifies the half space to which i belongs if evaluating the plane equation of the face

It is important to notice the difference between cam[1] and cam[2]. cam[1] is the largest change within an iteration of the actual increment. If the corrections in subsequent iterations all belonging to the same increment are 5,1,0.1, the value of cam[1] is 5. cam[2] is the largest temperature change within the increment, in the above example this is 6.1.

10 Verification examples.

The verification examples are simple examples suitable to test distinct features. They can be used to check whether the installation of CalculiX is correct, or to find examples when using a new feature. All verification examples are stored in ccx_2.8p2.test.tar.bz2. The larger fluid examples can be found in ccx_2.8p2.testfluid.tar.bz2.

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