ElmerSolver Manual

CSC – IT Center for Science

April 30, 2009

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About ElmerSolver Manual

The ElmerSolver Manual is part of the documentation of Elmer finite element software. ElmerSolver Manual describes the Elmer Solver options common for all specific equation solvers. The different equations solver options are described separately in Elmer Models Manual. The ElmerSolver Manual is best used as a reference manual rather than a concise introduction to the matter.

The present manual corresponds to Elmer software version 6.0 for Windows NT and Unix platforms. Latest documentations and program versions of Elmer are available (or links are provided) at `http://www.csc.fi/elmer`.

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Chapter 1

Structure of the Solver Input File

1.1 Introduction

Solving partial differential equation (PDE) models with the solver of Elmer requires that a precise description of the problem is given using the so-called solver input file, briefly referred to as the sif file. This file contains user-prepared input data which specify the location of mesh files and control the selection of physical models, material parameters, boundary conditions, initial conditions, stopping tolerances for iterative solvers, etc. In this chapter, the general structure of the file is described. We explain how the input data is organized into different sections and describe the general keyword syntax which is used in these sections to define the values of various model parameters and to control the solution procedures.

In the case of simple problem setups the solver input file may be written automatically by the preprocessor of Elmer software, so that knowing the solver input file format may be unnecessary. Creating a more complicated setup, or using keywords introduced by the user, however, requires the knowledge of the file format and keyword syntax.

In the following the general structure of the input file is first illustrated by using simple examples, without trying to explain all possibilities in an exhaustive manner. We then describe the keyword syntax in more detail, showing also how model parameters whose values depend on solution fields can be created. The later chapters of this manual, and Elmer Models Manual, which focuses on describing the PDE models Elmer can handle, provide more detailed material on specific issues. Elmer Tutorial Manual also gives complete examples of solver input files.

1.2 The sections of solver input file

The material of the solver input file is organized into different sections. Each section is generally started with a row containing the name of the section, followed by a number of keyword commands, and ended with a row containing the word `End`. The names for starting new sections are

- `Header`
- `Simulation`
- `Constants`
- `Body n`
- `Material n`
- `Body Force n`
- `Equation n`

- `Solver n`
- `Boundary Condition n`
- `Initial Condition n`

Here `n` associated with the section name represents an integer identifier needed for distinguishing between sections of the same type. A basic keyword command included in a section is nothing more than a statement which sets the value of a keyword with an equal sign.

In the following we describe how the sections are basically arranged without trying to explain all possibilities in an exhaustive manner. The later chapters of this manual and Elmer Models Manual provide more detailed material on specific issues. Elmer Tutorial Manual also gives complete examples of solver input files.

Header section. The location of mesh files is usually given in the header section. Often this is also the only declaration given in the header section. If the Elmer mesh files (see Appendix A) are located in the directory ./1d, the header section may simply be

```
Header
  Mesh DB "." "1d"
End
```

Note that separate equations can nevertheless be discretized using different meshes if the location of mesh files is given in the solver section described below.

Simulation section. The simulation section is used for giving general information that is not specific to a particular PDE model involved in the simulation. This information describes the coordinate system used, indicates whether the problem is stationary or evolutionary, defines the file names for outputting, etc. Without trying to describe many possibilities and the details of commands, we only give the following simple example:

```
Simulation
  Coordinate System = "Cartesian 1D"
  Coordinate Mapping(3) = 1 2 3
  Simulation Type = Steady State
  Steady State Max Iterations = 1
  Output Intervals(1) = 1
  Post File = "1dheat.ep"
  Output File = "1dheat.dat"
End
```

Constants section. The constants section is used for defining certain physical constants. For example the gravity vector and the Stefan-Boltzmann constant may be defined using the commands

```
Constants
  Gravity(4) = 0 -1 0 9.82
  Stefan Boltzmann = 5.67e-08
End
```

If the constants are not actually needed in the simulation, this section can also be left empty.

Body, material, body force and initial condition sections. The Elmer mesh files contain information on how the computational region is divided into parts referred to as bodies. A body section associates each body with an equation set, material properties, body forces, and initial conditions by referring to definitions given in a specified equation section, material section, body force section, and initial condition section. To manage to do this, the different sections of the same type are distinguished by integer identifiers that are parts of the section names. Note that the integer in the body section name is an identifier for the body itself.

For example, one may define

```
Body 1
  Material = 1
  Body Force = 1
  Equation = 1
  Initial Condition = 2
End
```

Material properties, body forces, an equation set, and initial conditions are then defined in the material section

```
Material 1
  ...
End
```

the body force section

```
Body Force 1
  ...
End
```

the equation section

```
Equation 1
  ...
End
```

and the initial condition section

```
Initial Condition 2
  ...
End
```

What material properties and body forces need to be specified depends on the mathematical models involved in the simulation, and the initial condition section used for giving initial values is only relevant in the solution of evolutionary problems. We here omit the discussion of these very model-dependent issues; after reading this introductory chapter the reader should be able to understand the related documentation given in Elmer Models Manual, which focuses on describing the different mathematical models, while the contents of equation section will be described next.

Equation and solver sections. Equation section provides us a way to associate each body with a set of equation solvers. That is, if the set defined consists of more than one equation solver, several physical phenomena may be considered to occur simultaneously over the same region of space. Individual equation solvers are actually defined in solver sections, the contents of an equation section being basically a list of integer identifiers for finding the solver sections that define the solvers. The keyword commands given in the solver sections then control the selection of physical models, linearization procedures of nonlinear models, the selection of solution methods for resulting linear equations, convergence tolerances, etc.

For example, if only two solvers are needed, one may simply define a list of two solver identifiers

```
Equation 1
  Active Solvers(2) = 1 2
End
```

Then the solver definitions are read from the solver sections

```
Solver 1
  ...
End
```

and

```
Solver 2
  ...
End
```

Finally, we give an example of solver definitions, without trying to explain the commands at this point:

```
Solver 1
  Equation = "Poisson"
  Variable = "Potential"
  Variable DOFs = 1
  Procedure = "Poisson" "PoissonSolver"
  Linear System Solver = "Direct"
  Steady State Convergence Tolerance = 1e-06
End
```

Boundary condition section. Boundary condition sections define the boundary conditions for the different equations. The Elmer mesh files contain information on how the boundaries of the bodies are divided into parts distinguished by their own boundary numbers. The keyword `Target Boundaries` is used to list the boundary numbers that form the domain for imposing the boundary condition. For example the declaration

```
Boundary  Condition 1
  Target Boundaries(2) = 1 2
  ...
End
```

means that the boundary condition definitions that follow concern the two parts having the boundary numbers 1 and 2.

We finally note that some commands, such as comments started with the symbol ! and MATC expressions described below, may also be placed outside section definitions. An exception of this type is also the command

```
Check Keywords "Warn"
```

usually placed in the beginning of the input file. When this command is given, the solver outputs warning messages if the input file contains keywords that are not listed in the file of known keywords. If new keywords are introduced, misleading warning messages can be avoided by adding the new keywords to the keyword file `SOLVER.KEYWORDS`, located in the directory of the shared library files of ElmerSolver.

1.3 Keyword syntax

As already illustrated, a basic keyword command used in the solver input file is a statement which sets the value of a solution parameter with the equal sign. Such a command in its full form also contains the data type declaration; for example

```
Density = Real 1000.0
```

Valid data types generally are

- `Real`
- `Integer`
- `Logical`
- `String`
- `File`

If the keyword is listed in the keyword file `SOLVER.KEYWORDS`, the data type declaration may be omitted. Therefore, in the case of our example, we may also define

```
Density = 1000.0
```

The value of a keyword may also be an array of elements of specified data type, with the array size definition associated with the keyword. We recall our previous examples of the equation and boundary condition sections, where we defined two lists of integers using the commands

```
Active Solvers(2) = 1 2
```

and

```
Target Boundaries(2) = 1 2
```

Two-dimensional arrays are also possible and may be defined as

```
My Parameter Array(3,3) = Real 1 2 3 \
                               4 5 6 \
                               7 8 9
```

Defining parameters depending on field variables. Most solver parameters may depend on time, or on the field variables defined in the current simulation run. Such dependencies can generally be created by means of tabular data, MATC functions, or Fortran functions. MATC has the benefit of being an interpreted language, making an additional compilation step with a compiler unnecessary.

Simple interpolating functions can be created by means of tabular data. The following example defines the parameter `Density` the value of which depends on the variable `Temperature`:

```
Density = Variable Temperature
  Real
    0    900
    273 1000
    300 1020
    400 1000
End
```

This means that the value of `Density` is 900 when `Temperature` is 0, and the following lines are interpreted similarly. Elmer then uses linear interpolation to approximate the parameter for argument values not given in the table. If the value of the independent variable is outside the data set, the first or the last interpolating function which can be created from the tabulated values is used to extrapolate the value of the parameter.

If the field variable has several independent components, such as the components of displacement vector, the independent components may be used as arguments in a function definition. For example, if a three-component field variable is defined in a solver section using the commands

```
Variable = "Displ"
Variable DOFs = 3
```

then the solver of Elmer knows, in addition to the three-component vector `Displ`, three scalar fields `Displ 1`, `Displ 2` and `Displ 3`. These scalar fields may be used as independent variables in parameter definitions, and used in the definitions of initial and boundary conditions, etc.

More complicated functions can be defined using MATC language. Here the basic usage of MATC in connection with the solver input file is illustrated; for an additional documentation, see a separate manual for MATC. For example, one may define

```
Density = Variable Temperature
  MATC "1000*(1-1.0e-4*(tx-273))"
```

This means that the parameter `Density` depends on the value of `Temperature` as

$$\rho = \rho_0(1 - \beta(T - T_0)), \tag{1.1}$$

with $\rho_0 = 1000, \beta = 10^{-4}$ and $T_0 = 273$. Note that the value of the independent variable is known as `tx` in the MATC expression.

If the independent variable has more than one component, the variable `tx` will contain all the components in values `tx(0)`,`tx(1)`,...,`tx(n-1)`, where `n` is the number of the components of the independent variable. A MATC expression may also take several scalar arguments; one may define, for example,

```
My Parameter = Variable Time, Displ 1
  Real MATC "..."
```

The values of the scalar fields `Time` and `Displ 1` can then be referred in the associated MATC expression by the names `tx(0)` and `tx(1)`, respectively.

In addition to using MATC functions, Fortran 90 functions may also be used to create parameter definitions, etc. In the same manner as MATC functions are used, we may define

```
Density  = Variable Temperature
  Procedure "filename" "proc"
```

In this case the file "filename" should contain a shareable .so (Unix) or .dll (Windows) code for the user function whose name is "proc". The call interface for the Fortran function is as follows

```
FUNCTION proc( Model, n, T ) RESULT(dens)
  USE DefUtils)
  IMPLICIT None
  TYPE(Model_t) :: Model
  INTEGER :: n
  REAL(KIND=dp) :: T, dens

  dens = 1000*(1-1.0d-4(T-273.0d0))
END FUNCTION proc
```

The Model structure contains pointers to all information about the model, and may be used to obtain field variable values, node coordinates, etc. The argument n is the index of the node to be processed, and T is the value of the independent variable at the node. The function should finally return the value of the dependent variable.

The independent variable can also be composed of several independent components. We may thus define

```
Density = Variable Coordinate
  Procedure "filename" "proc"
```

Now the argument T in the Fortran function interface should be a real array of three values, which give the x,y and z coordinates of the current node.

Parameterized keyword commands. The solver input file also offers possibilities for creating parameterized commands that utilize MATC. In the solver input file an expression following the symbol $ is generally interpreted to be in MATC language. If the solver input file contains the lines

```
$solvertype = "Iterative"
$tol = 1.0e-6
```

then one may define, e.g.,

```
Solver 1
  ...
  Linear System Solver = $solvertype
  Linear System Convergence Tolerance = $tol
  ...
End

Solver 2
  ...
  Linear System Solver = $solvertype
  Linear System Convergence Tolerance = $100*tol
  ...
End
```

Chapter 2

Finite Element Utilities

2.1 Introduction

This section decribes Elmer Solver utilities related directly to Finite Element Method (FEM). Finite element method is a common procedure to solve differential and integral equations numerically.

2.2 Theory

For higher-order finite elements see the separate chapter.

Chapter 3

Solution Methods for Linear Systems

3.1 Introduction

Discretization and linearization of a system of partial differential equations leads to linear systems

$$Ax = b, \tag{3.1}$$

where A and b are of orders $n \times n$ and $n \times 1$, respectively. A specific feature of the coefficient matrix A resulting from the finite element discretization is that the matrix is sparse, i.e. only a few of the matrix entries in each row differ from zero. In many applications the system can also have a very large order n, so that the chief part of the computation time in performing the simulation is typically spent by solvers for the linear systems.

Solution methods for linear systems fall into two large categories: direct methods and iterative methods. Direct methods determine the solution of the linear system exactly up to a machine precision. They perform in a robust manner leading to the solution after a predetermined number of floating-point operations. Nevertheless, the drawback of direct methods is that they are expensive in computation time and computer memory requirements and therefore cannot be applied to the solution of linear systems of very large order. The efficient solution of large systems requires generally the use of iterative methods which work by generating sequences of improving approximate solutions.

ElmerSolver provides access to both direct and iterative methods. The iterative methods available fall into two main categories: preconditioned Krylov subspace methods and multilevel methods. Iteration methods that combine the ideas of these two approaches may also be constructed. Such methods may be very efficient leading to a solution after a nearly optimal number of operation counts.

The development of efficient solution methods for linear systems is still an active area of research, the amount of literature on the topic being nowadays vast. The aim of the following discussion is to provide the user the basic knowledge of the solution methods available in ElmerSolver. The detailed description of methods is omitted. For a more comprehensive treatment the reader is referred to references mentioned.

3.2 Direct methods

A linear system may be solved in a robust way by using direct methods. There are two different options for direct methods in ElmerSolver. The default method utilizes the well-known LAPACK collection of subroutines for band matrices. In practice, this solution method can only be used for the solution of small linear systems as the operation count for this method is of order n^3.

The other direct solver employs the UMFPACK routines to solve sparse linear systems [1]. UMFPACK uses the Unsymmetric MultiFrontal method. In practice it may be the most efficient method for solving 2D problems as long as there is enough memory available.

It should be noted that the success of the direct solvers depends very much on the bandwidth of the sparse matrix. In 3D these routines therefore usually fail miserably.

3.3 Preconditioned iteration methods

ElmerSolver contains a set of Krylov subspace methods for the iterative solution of linear systems. These methods may be applied to the solution large linear systems but rapid convergence generally requires the use of preconditioning.

3.3.1 Krylov subspace methods

The Krylov subspace methods available in ElmerSolver are

- Conjugate Gradient (CG)
- Conjugate Gradient Squared (CGS)
- Biconjugate Gradient Stabilized (BiCGStab)
- Transpose-Free Quasi-Minimal Residual (TFQMR)
- Generalized Minimal Residual (GMRES)

Both real and complex systems can be solved using these algorithms. For the detailed description of these methods see [3] and [4].

A definite answer to the question which the best iteration method for a particular case is cannot be given. In the following only some remarks on the applicability of the methods are made.

The CG method is an ideal solution algorithm for the cases where the coefficient matrix A is symmetric and positive definite. The other methods may also be applied to the cases where A is non-symmetric. It is noted that the convergence of the CGS method may be irregular. The BiCGStab and TFQMR methods are expected to give smoother convergence. The GMRES method generates iterates satisfying an optimality condition, but the computational work and computer memory requirements of the method increase as the number of iterations grows. In practice one often has to use a restarted version of this method based on restarting the iteration after m iterations. The convergence of the method may however be considerably slower than that of full GMRES. The choice of m has to be controlled by the user. Unfortunately, general guidelines for determining a reasonable value for m cannot be given as this value is case-dependent.

3.3.2 Preconditioning strategies

The performance of iteration methods depends greatly on the spectrum of the coefficient matrix A. The rate at which an iteration method converges can often be improved by transforming the original system into an equivalent one that has more favorable spectral properties. This transformation is called preconditioning and a matrix which determines the transformation is called a preconditioner.

In ElmerSolver preconditioning is done by transforming (4.1) into the system

$$AM^{-1}z = b, \tag{3.2}$$

where the preconditioner M is an approximation to A and z is related to the solution x by $z = Mx$. In practice, the explicit construction of the inverse M^{-1} is not needed, since only a subroutine that for given v returns a solution u to the system

$$Mu = v \tag{3.3}$$

is required.

ElmerSolver provides several preconditioning strategies. These include Jacobi preconditioning and incomplete factorization preconditioners. The preconditioning step (3.3) may even be defined in terms of some iteration method for the system (3.3) with $M = A$. This possibility is considered in Section 3.4.3 below.

The Jacobi preconditioner is simply based on taking M to be the diagonal of A. More sophisticated preconditioners may be created by computing incomplete LU factorizations of A. The resulting preconditioners are referred to as the ILU preconditioners. This approach gives the preconditioner matrix M in the form $M = LU$ where L and U are lower and upper triangular with certain elements that arise in the factorization process ignored.

There are several ways to choose a set of matrix positions that are allowed to be filled with nonzero elements. ILU preconditioners of fill level N referred to as the ILU(N) preconditioners are built so that ILU(0) accepts nonzero elements in the positions in which A has nonzero elements. ILU(1) allows nonzero elements in the positions that are filled if the first step of Gaussian elimination is performed for A. ILU(2) accepts fill in positions that are needed if the next step of Gaussian elimination is performed with ILU(1) factorization, etc.

Another strategy is based on numerical tolerances. The resulting preconditioner is referred to as the ILUT preconditioner. In the creation of this preconditioner Gaussian elimination is performed so that elements of a given row of the LU factorization are obtained but only elements whose absolute value (scaled by the norm of all values of the row) is over a given threshold value are accepted in the preconditioner matrix.

Obviously, the additional computation time that is spent in creating the preconditioner matrix and solving systems of the type (3.3) should be compensated by faster convergence. Finding an optimal ILU preconditioner for a particular case may require the use of trial and error. Start with ILU(0) and try to increase the fill level N. As N increases, more and more elements in the incomplete LU factorization of the coefficient matrix are computed, so the preconditioner should in principle be better and the number of iterations needed to obtain a solution should decrease. At the same time the memory usage grows rapidly and so does the time spent in building the preconditioner matrix and in applying the preconditioner during iterations. The same applies to the ILUT preconditioner with decreasing threshold value.

3.4 Multilevel methods

A class of iterative methods referred to as multilevel methods provides an efficient way to solve large linear systems. For certain class of problems they perform nearly optimally, the operation count needed to obtain a solution being nearly of order n. Two different multilevel-method approaches are available in ElmerSolver, namely the geometric multigrid (GMG) and algebraic multigrid (AMG).

3.4.1 Geometric multigrid

Given a mesh $\mathcal{T}_1$ for the finite element discretization of problem the geometric multigrid method utilizes a set of coarser meshes $\mathcal{T}_k$, $k = 2, ..., N$ to solve the linear system arising from the discretization. One of the fundamental ideas underlying the method is based on the idea of coarse grid correction. That is, a coarser grid is utilized to obtain an approximation to the error in the approximate solution of the linear system. The recursive application of this strategy leads us to multigrid methods.

To utilize different meshes multigrid methods require the development of methods for transferring vectors between fine and coarse meshes. Projection operators are used to transfer vectors from a fine mesh $\mathcal{T}_k$ to a coarse mesh $\mathcal{T}_{k+1}$ and will be denoted by I_k^{k+1}, while interpolation operators I_{k+1}^k transfer vectors from a coarse mesh to a fine mesh.

The multigrid method is defined by the following recursive algorithm: Given A, b and an initial guess y for the solution of the system $Ax = b$ set $i = 1$ and do the following steps

1. If $i = N$, then solve the system $Ax = b$ by using the direct method and return.
2. Do pre-smoothing by applying some iterative algorithm for a given number of times to obtain a new approximate solution y.
3. Perform coarse grid correction by starting a new application of this algorithm with $A = I_i^{i+1} A I_{i+1}^i$, $b = I_i^{i+1}(Ay - b)$, $i = i + 1$ and the initial guess $e = 0$.
4. Compute a new approximate solution by setting $y = y + I_{i+1}^i e$
5. Do post-smoothing by applying some iterative algorithm for a given number of times to obtain a new approximate solution y.
6. If the solution has not yet converged, go to point 2.

In ElmerSolver one may choose the Jacobi, CG or BiCGStab algorithm as the method for smoothing iterations.

The full success of multigrid methods is based on the favorable combination of the properties of basic iteration methods and methods for transferring vectors between meshes. The smoothing iterations give rapid convergence for oscillatory solution components while coarse grid correction entails an efficient solution method for smooth solution components. For a comprehensive introduction to the geometric multigrid method the reader is referred to [2].

3.4.2 Algebraic multigrid

In many cases the geometric multigrid may not be applied because we do not have the luxury of having a set of appropriate hierarchical meshes. The alternative is the algebraic multigrid (AMG) method which uses only the matrix A to construct the projectors and the coarse level equations. AMG is best suited for symmetric and positive semidefinite problems. For other types of problems the standard algorithm may fail. For more information on AMG see reference [5].

The AMG method has two main phases. The set-up phase includes the recursive selection of the coarser levels and definition of the transfer and coarse-grid operators. The solution phase uses the resulting components to perform a normal multigrid cycling until a desired accuracy is reached. The solution phase is similar to that of the GMG.

Note that the AMG solvers in ElmerSolver are not fully mature. They may provide good solutions for some problems while desperately failing for others.

Classical Ruge-Stüben algorithm

The coarsening is performed using a standard Ruge-Stüben coarsening algorithm. The possible connections are defined by the entries in the matrix A. The variable i is strongly coupled to another variable j if

$$a_{ij} < -c_- \max |a_{ik}| \quad \text{or} \quad a_{ij} > c_+ \max |a_{ik}|, \tag{3.4}$$

where $0 < c_- < 1$ and $0 < c_+ < 1$ are parameters. Typically $c_- \approx 0.2$ and $c_+ \approx 0.5$. Once the negative (P^-) and positive (P^+) strong couplings have been determined the variables are divided into coarse (C) and fine (F) variables using the standard coarsening scheme.

The interpolation matrix may be constructed using the C/F-splitting and the strong couplings of the matrix. The interpolation of coarse nodes is simple as they remain unchanged. The interpolation of fine nodes starts from the fact the smooth error e must roughly satisfy the condition $Ae = 0$ or

$$a_{ii}e_i + \sum_{j \neq i} a_{ij}e_j = 0. \tag{3.5}$$

By manipulation

$$a_{ii}e_i + \alpha_i \sum_{j \in C \cap P_i^-} a_{ij}e_j + \beta_i \sum_{j \in C \cap P_i^+} a_{ij}e_j = 0, \tag{3.6}$$

where

$$\alpha_i = \frac{\sum_{j \in P_i^-} a_{ij}}{\sum_{j \in C \cap P_i^-} a_{ij}} \quad \text{and} \quad \beta_i = \frac{\sum_{j \in P_i^+} a_{ij}}{\sum_{j \in C \cap P_i^+} a_{ij}}. \tag{3.7}$$

The interpolation thus becomes

$$e_i = \sum_{j \in C \cap P_i} w_{ij}e_j \quad \text{with} \quad w_{ij} = \begin{cases} -\alpha_i a_{ij}/a_{ii}, & j \in P_i^-, \\ -\beta_i a_{ij}/a_{ii}, & j \in P_i^+. \end{cases} \tag{3.8}$$

This is known as *direct interpolation*. It may be modified by using also the strong F-nodes in the interpolation. This means that in formula (3.5) the following elimination is made for each $j \in F \cap P_i$

$$e_j \to -\sum_{k \in C \cap P_j} a_{jk}e_k/a_{jj}. \tag{3.9}$$

This is known as *standard interpolation*. In practice it means that the number of nodes used in the interpolation is increased. This may be important to the quality of the interpolation particularly if the number of direct C-neighbors is small.

After the interpolation weights have been computed the smallest coefficients may be truncated if they are small, *i.e.*, $w_j < c_w \max |w_k|$, where $c_w \approx 0.2$. The other values must accordingly be increased so that the sum of weights remains constant. The truncation is essential in preventing the filling of the coarse level matrices.

Cluster multigrid

There is also an implementation of the agglomeration or cluster multigrid method. It is a variant of the algebraic multigrid method. In this method the components are grouped and the coarse-level matrices are created simply by summing up the corresponding rows and columns. In other words, the projection matrix includes just ones and zeros.

The cluster multigrid method should be more robust for problems where it is difficult to generate an optimal projection matrix. However, for simple problems it is usually beaten by the standard Ruge-Stüben method.

3.4.3 Preconditioning by multilevel methods

Multilevel methods are iteration methods on their own but they can also be applied as preconditioners for the Krylov subspace methods. This preconditioning approach corresponds to taking $M = A$ in (3.3) and performing an inaccurate solution of the resulting system using multilevel methods to obtain u. A rather mild stopping criterion may be used in this connection. Preconditioning by multilevel methods may lead to very efficient solution methods for large linear systems.

3.5 Keywords related to linear system solvers

The following keywords may be given in Solver section of the solver input file (.sif file).

`Linear System Solver` String

Using this keyword the type of linear system solver is selected. This keyword may take the following values:

- `Direct`
- `Iterative`
- `Multigrid`

Here `Iterative` and `Multigrid` refer to the Krylov and multilevel methods, respectively.

`Linear System Direct Method` String

If the value of the `Linear System Solver` keyword is set to be `Direct`, one may choose a band matrix solver with the value `Banded` or a sparse matrix solver with the value `Umfpack`. The default is `Banded`.

`Linear System Iterative Method` String

If the value of the `Linear System Solver` keyword is set to be `Iterative`, one should choose a Krylov method by setting the value of this keyword to be one of the following alternatives:

- `CG`
- `CGS`
- `BiCGStab`
- `TFQMR`

- `GMRES`

See also the `MG Smoother` keyword.

`Linear System GMRES Restart` `Integer [10]`
The restart parameter m for the GMRES method may be given using this keyword.

`Linear System Preconditioning` `String`
A preconditioner for the Krylov methods may be declared by setting the value of this keyword to be one of the following alternatives:

- `None`
- `Diagonal`
- `ILUn`, where the literal `n` may take values 0,1,...,9.
- `ILUT`
- `Multigrid`

See also the `MG Preconditioning` keyword.

`Linear System ILUT Tolerance` `Real [0.0]`
This keyword is used to define the value of the numerical tolerance for the ILUT preconditioner.

`Linear System Convergence Tolerance` `Real [0.0]`
This keyword is used to define a stopping criterion for the Krylov methods. The approximate solution is considered to be accurate enough if the iterate satisfies

$$\frac{||Ax-b||}{||b||} \leq \epsilon$$

where ϵ is the value of this keyword. See also `MG Tolerance`.

`Linear System Max Iterations` `Integer [0]`
This keyword is used to define the maximum number of the iterations the Krylov methods are permitted to perform. If this limit is reached and the approximate solution does not satisfy the stopping criterion, ElmerSolver either continues the run using the current approximate solution as the solution of the system or aborts the run depending on the value of `Linear System Abort Not Converged` keyword. See also `MG Max Iterations` keyword.

`Linear System Abort Not Converged` `Logical [True]`
If the value of this keyword is set to be `True`, ElmerSolver aborts the run when the maximum number of iterations the algorithm is permitted to perform is reached and the approximate solution does not satisfy the stopping criterion. Otherwise the run will be continued using the current approximate solution as the solution of the system (this may lead to troubles at later steps of computation).

`Linear System Residual Output` `Integer [1]`
By default the iterative algorithms display the value of the (scaled) residual after each iteration step. Giving a value $n > 1$ for this keyword may be used to display the residual only after every n iterations. If the value 0 is given, the residual output is disabled.

`Linear System Precondition Recompute` `Integer [1]`
By default the ElmerSolver computes the preconditioner when a new application of iterative algorithm is started. If the value of this keyword is set to be `n`, the preconditioner is computed only after n successive subroutine calls for linear systems arising from same source. This may speed up the solution procedure especially in cases where the coefficient matrix does not change much between successive subroutine calls. On the other hand if the coefficient matrix has changed significantly, the preconditioner may not be efficient anymore.

`Optimize Bandwidth` `Logical [True]`
: If the value of this keyword is set to be `True`, the Cuthill-McKee bandwidth optimization scheme is used to order the unknowns in such a way that band matrices can be handled efficiently. The bandwidth optimization is recommended when the direct solver or incomplete factorization preconditioners are used.

The keywords beginning with `MG` are activated only if either the `Linear System Solver` or `Linear System Preconditioning` keyword has the value `Multigrid`. If a multigrid method is used as the linear system solver, some keywords starting with `MG` may be replaced by corresponding keywords starting with phrase `Linear System`. It should be noted that in the case of a multigrid solver there are some limitations to what values the keywords starting with the phrase `Linear System` may take, see below.

`MG Levels` `Integer [1]`
: This keyword is used to define the number of levels for the multigrid method.

`MG Equal Split` `Logical [False]`
: A hierarchy of meshes utilized by the multigrid method may be generated automatically by setting the value of this keyword to be `True`. The coarsest partitioning must be supplied by the user and is declared in the usual way in the Header section of the solver input file. The other meshes are obtained using an equal division of the coarser mesh. The solution of the problem will be sought for the finest mesh.

`MG Mesh Name` `File`
: A hierarchy of meshes utilized by the multigrid method may be supplied by the user. A base name of the mesh directories is declared using this keyword. The names of mesh directories must be composed of the base name appended with a level number such that if the base name is `mgridmesh`, the mesh directories should have names `mgridmesh1`, `mgridmesh2`, etc. The meshes are numbered starting from the coarsest mesh. In addition, the finest mesh must be declared in the Header section of the solver input file. It should be noted that the `MG Equal Split keyword` must be set to be `False` to enable the use of user-supplied meshes.

`MG Max Iterations` `Integer [0]`
: If a multigrid method is used as a preconditioner for the Krylov methods, the value of this keyword defines the maximum number of iterations the multigrid method is allowed to perform to solve the preconditioning equation (3.3). Usually one or two iterations are sufficient. If a multigrid method is the linear system solver, the use of this keyword is similar to that of the `Linear System Max Iterations` keyword.

`MG Convergence Tolerance` `Real [0.0]`
: If a multigrid method is used as a preconditioner for the Krylov methods, this keyword defines the solution accuracy for the preconditioning equation (3.3). This keyword is not usually needed if the `MG Max Iterations` keyword has a small value. If a multigrid method is the linear system solver, the use of this keyword is similar to that of the `Linear System Convergence Tolerance` keyword.

`MG Smoother` `String`
: This keyword defines the algorithm for pre- and post-smoothing. It may take one of the following values:

  - `Jacobi`
  - `CG`
  - `BiCGStab`

  If the linear system solver is a multigrid method, the `Linear System Iterative Method` keyword may be used instead of this keyword, but only the three algorithms mentioned here can be applied.

`MG Pre Smoothing Iterations` `Integer [0]`
This keyword defines the number of pre-smoothing iterations.

`MG Post Smoothing Iterations` `Integer [0]`
This keyword defines the number of post-smoothing iterations.

`MG Preconditioning` `String`
This keyword declares the preconditioner for the algorithm which is used in smoothing iterations. It may take one of the following values:

- `None`
- `ILUn`, where the literal `n` may take values 0,1,...,9.
- `ILUT`

Note that this keyword is not related to using multigrid method as a preconditioner. It is also noted that preconditioning the smoothing algorithms does not seem to work well if a multigrid method is used as a preconditioner for Krylov methods.

`MG ILUT Tolearance` `Real [0.0]`
This keyword defines the numerical tolerance for the ILUT preconditioner in connection with smoothing iterations.

The keywords for the algebraic multigrid solver are in a large part the same as for the geometric multigrid. There are however some keywords that are related only to AMG.

`MG Lowest Linear Solver Limit` `Integer`
This value gives a lower limit for the set of coarse nodes after which the recursive multilevel routine is terminated. A proper value might be around 100.

`MG Recompute Projector` `Logical`
This flag may be used to enforce recomputation of the projector each time the algebraic multigrid solver is called. The default is `False` as usually the same projector is appropriate for all computations.

`MG Eliminate Dirichlet` `Logical`
At the highest level the fixed nodes may all be set to be coarse since their value is not affected by the lower levels. The default is `True`

`MG Eliminate Dirichlet Limit` `Real`
Gives the maximum fraction of non-diagonal entries for a Dirichlet node.

`MG Smoother` `String`
In addition to the selection for the GMG option `sor` (symmetric over relaxation) is possible.

`MG SOR Relax` `String`
The relaxation factor for the SOR method. The default is 1.

`MG Strong Connection Limit` `Real`
The coefficient c_- in the coarsening scheme. Default is 0.25.

`MG Positive Connection Limit` `Real`
The coefficient c_+ in the coarsening scheme. Default is 1.0.

`MG Projection Limit` `Real`
The coefficient c_w in the truncation of the small weights. The default is 0.1.

`MG Direct Interpolate` `Logical`
Chooses between direct and standard interpolation. The default is `False`.

`MG Direct Interpolate Limit` `Integer`
The standard interpolation may also be applied to nodes with only a small number of coarse connection. This gives the smallest number of nodes for which direct interpolation is used.

Finally, there are also some keywords related only to the clustering multigrid.

`MG Cluster Size` Integer
: The desired choice of the cluster. Possible choices are 2,3,4,5,... and zero which corresponds to the maximum cluster.

`MG Cluster Alpha` Real
: In the clustering algorithm the coarse level matrix is not optimal for getting the correct convergence. Tuning this value between 1 and 2 may give better performance.

`MG Strong Connection Limit` Real
: This is used similarly as in the AMG method except it is related to positive and negative connections alike.

`MG Strong Connection Minimum` Integer
: If the number of strong connections with the given limit is smaller than this number then increase the set of strong connection if available connections exist.

3.6 Implementation issues

3.6.1 The sparse matrix storage

To be efficient, iteration methods require that a matrix-vector product for sparse matrices is efficiently implemented. A special storage scheme called the Compressed Row Storage (CRS) [3] is used in ElmerSolver to store only those matrix coefficients that differ from zero.

The matrix structure is defined in module `Types` as:

```
TYPE Matrix_t
   ...
  INTEGER :: NumberOfRows

  REAL(KIND=dp),  POINTER :: Values(:)
  INTEGER, POINTER :: Rows(:), Cols(:), Diag(:)
   ...
END TYPE Matrix_t
```

The matrix type has several additional fields, but the basic storage scheme can be implemented using the fields shown. The array `Values` is used to store the nonzero elements of the coefficient matrix. The array `Cols` contains the column numbers for the elements stored in the array `Values`, while the array `Rows` contains indices to elements that start new rows. In addition, `Row(n+1)` gives the number of nonzero matrix elements + 1. The array `Diag` is used to store the indices of the diagonal elements.

For example, to go through the matrix row by row the following loop may be used

```
USE Types
TYPE(Matrix_t), POINTER :: A
REAL(KIND=dp):: val
INTEGER :: i, j, row, col

DO i=1, A % NumberOfRows
  PRINT *, 'Diagonal element for row ', i, ' is ', A % Values( A % Diag(i) )
  DO j=A % Rows(i), A % Rows(i+1)-1
     row = i
     col = A % Cols(j)
     val = A % Values(j)
     PRINT *, 'Matrix element at position: ', row,col, ' is ', val
  END DO
END DO
```

3.6.2 Subroutine calls

Most of the functionality of the sparse linear system solver of the ElmerSolver is available by using the function call

```
  Norm = DefaultSolve().
```

The return value `Norm` is a norm of the solution vector.

Sometimes it may be convenient to modify the linear system before solving it. A Fortran function which performs this modification can be written by the user with the name of the function being declared in the solver input file. For example, this technique may be used to define a user-supplied linear system solver.

If the name of the user-supplied Fortran function is `proc` and it can be found in the file having the name `Filename`, the declaration

```
Before Linsolve  File Filename proc
```

in the solver input file has the effect that the function will be called just before the default call of linear system solver. The arguments the function can take are fixed and are declared as

```
   FUNCTION proc( Model, Solver, A,  b, x, n, DOFs, Norm ) RESULT(stat)
      USE SolverUtils
      TYPE(Model_t)  :: Model
      TYPE(Solver_t) :: Solver
      TYPE(Matrix_t), POINTER :: A
      REAL(KIND=dp) :: b(:), x(:), Norm
      INTEGER :: n, DOFs, stat
      ...
   END FUNCTION proc
```

Here the Model structure contains the whole definition of the elmer run. The Solver structure contains information for the equation solver from which this linear system originates. The coefficient matrix `A` is in CRS format, `b` is the right-hand side vector, and `x` contains the previous solution. The argument `n` is the number of unknowns, and `DOFs` is the number of unknowns at a single node.

If the return value from this function is zero, the (possibly) modified linear system is solved after the return. If the return value is 1, the linear system is assumed to be already solved and the vector `x` should contain the result. It is noted that the user-supplied Fortran function may also call the default linear equation solver within the function, i.e. one may write the subroutine call

```
   CALL SolveLinearSystem( A, b, x, Norm, DOFs, Solver )
```

Here `A` and `b` may be modified so that the linear system which is solved need not be same as the input system.

In a similar way the user may also supply a user-defined Fortran function which will be called just after the solution of linear system. This is done using the declaration

```
After Linsolve  File Filename proc
```

in the solver input file. The arguments of this function are the same as for a function in the context of `Before Linsolve` keyword.

Bibliography

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[4] R.W. Freund. A transpose-free quasi-minimal residual algorithm for non-hermitian linear systems. *SIAM J. Sci. Comput.*, 14:470–482, 1993.

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Chapter 4

Nonlinear System Options

4.1 Introduction

Numerical methods in linear algebra are usually intended for the solution of linear problems. However, there are many problems which are not linear in nature. The nonlinearity may a intrinsic characteristics of the equation, such as is the case with intertial forces in the Navier-Stokes equation. The nonlinerity might also a result of nonlinear material parameters that depend on the solution. What ever the reason for nonlinearity the equations in Elmer are always first linearized to the form

$$A(u_{i-1})u_i = b(u_{i-1}), \tag{4.1}$$

where i refers to the iteration cycle.

How the equations are linearized varies from solver toanother. For example, in the Navier-Stokes solver there are tow different methods – the Picard linearization and the Newton linearization that may be used. Also a hybrid scheme where the Picard type of scheme is switched to the Newton kind of scheme when certain criteria are met is available. Therefore this section will not deal with the particular linearization technique of different solver but tries to give some light to the generic keywords that are available. Some keywords may also be defined in the Models Manual related to particular solvers.

In multiphysical simulations there are also a number of keywords related to the solution of coupled systems. Basically one may may define how many times a system of equations is solved repeatedly at maximum and how what are the convergence criteria of the individual solvers that must be met simulataneously.

4.2 Keywords related to solution of nonlinear systems

These keywords are located in the Solver section of each solver, if requited at all.

`Nonlinear System Convergence Measure` `String`

The change of solution between two consecutive iterations may be estimated by a number of different measures which are envoked by values `norm`, `solution` and `residual`. The default way of checking for convergence is to test the change of norm

$$\delta = 2 * ||u_i| - |u_{i-1}||/(|u_i| + |u_{i-1}|). \tag{4.2}$$

This measure is rather liberal since the norm of two solutions may be the same even though the solutions would not. Therefore it is often desirable to look at the norm of change,

$$\delta = 2 * |u_i - u_{i-1}|/(|u_i| + |u_{i-1}|). \tag{4.3}$$

The third choice is to use a backward norm of the residual where the old solution is used with the new matrix.

$$\delta = |Ax_{i-1} - b|/|b|. \tag{4.4}$$

In the current implementation this norm lags one step behind and therefore always performs one extra iteration.

`Nonlinear System Norm Degree` `Integer`
: The choice of norms used in the evaluation of the convergence measures is not self evident. The default is the $L2$ norm. This keyword may be used to replace this by Ln norm where value $n = 0$ corresponds to the infinity (i.e. maximum) norm.

`Nonlinear System Norm Dofs` `Integer`
: For vector valued field variables by default all components are used in the computation of the norm. However, sometimes it may be desirable only to use some of them. This keyword may be used to give the number of components used in the evaluation. For example, in the Navier-Stokes equations the norm is only taken in respect to the velocity components while pressure is omitted.

`Nonlinear System Convergence Absolute` `Logical`
: This keyword may be used to enforce absolute convergence measures rather than relative. The default is `False`.

`Nonlinear System Convergence Tolerance` `Real`
: This keyword gives a criterion to terminate the nonlinear iteration after the relative change of the norm of the field variable between two consecutive iterations is small enough $\delta < \epsilon$, where ϵ is the value given with this keyword.

`Nonlinear System Max Iterations` `Integer`
: The maxmimum number of nonlinear iterations the solver is allowed to do.

`Nonlinear System Newton After Iterations` `Integer`
: Change the nonlinear solver type to Newton iteration after a number of Picard iterations have been performed. If a given convergence tolerance between two iterations is met before the iteration count is met, it will switch the iteration type instead. This applies only to some few solvers (as the Navier-Stokes) where different linearization strategies are available.

`Nonlinear System Newton After Tolerance` `Real`
: Change the nonlinear solver type to Newton iteration, if the relative change of the norm of the field variable meets a tolerance criterion:

$$\delta < \epsilon,$$

where ϵ is the value given with this keyword.

`Nonlinear System Relaxation Factor` `Real`
: Giving this keyword triggers the use of relaxation in the nonlinear equation solver. Using a factor below unity is sometimes required to achive convergence of the nonlinear system. Typical values range between 0.3 and unity. If one must use smaller values for the relaxation factor some other methods to boost up the convergence might be needed to improve the convergence. A factor above unity might rarely speed up the convergence. Relaxed variable is defined as follows:

$$u_i^{'} = \lambda u_i + (1 - \lambda) u_{i-1},$$

where λ is the factor given with this keyword. The default value for the relaxation factor is unity.

Many of the keywords used to control the `Nonlinear System` have a corresponding keyword for the Steady State. Basically the operation is similar except the reference value for the current solution u_i is the last converged value of the nonlinear system before starting a new loosely coupled iteration cycle. Otherwise the explanations given above are valid.

`Steady State Convergence Measure` `String`

`Steady State Norm Degree` `Integer`

`Steady State Norm Dofs` `Integer`

`Steady State Convergence Tolerance` `Real`

`Steady State Relaxation Factor` `Real`

Additionally these keywords are located in the `Simulation` section of the command file.

`Steady State Max Iterations` `Integer`
: The maximum number of coupled system iterations. For steady state analysis this means it litelarly, for transient analysis this is the maximum number of iterations within each timestep.

`Steady State Min Iterations` `Integer`
: Sometimes the coupling is such that nontrivial solutions are obtained only after some basic cycle is repeated. Therefore the user may sometimes need to set also the minimum number of iterations. Sometimes the steady state loop is also used in a dirty way to do some systematic procedures – for example computing the capacitance matrix, or lumped elastic springs. Then this value may be set to an a priori known constant value.

Chapter 5

Integration of time-dependent systems

5.1 Introduction

Solving time-dependent systems is becoming more and more common in various branches of computational science, as the computer resources grow steadily. ElmerSolver may be adapted to solve such systems. The first order time derivatives may be discretizated by using the following methods:

- the Crank-Nicolson method
- the Backward Differences Formulae (BDF) of several orders

In the case of the first order BDF scheme adaptive time-stepping strategy may also be used.

The second order time derivatives are approximated by either using the Bossak method or reformulating the second order equations as equivalent systems of first order equations.

5.2 Time discretization strategies

Consider the numerical solution of the evolutionary field equation

$$\frac{\partial \phi}{\partial t} + \mathcal{K}\phi = f, \tag{5.1}$$

where the differential operator $\mathcal{K}$ does not involve differentiation with respect to time t and f is a given function of spatial coordinates and time. The spatial discretization of (5.1) leads to the algebraic equations

$$M\frac{\partial \Phi}{\partial t} + K\Phi = F, \tag{5.2}$$

where M, K and F result from the discretization of the identity operator, the operator $\mathcal{K}$ and f, respectively. The vector Φ contains the values of the unknown field ϕ at nodes.

The applications of the first three BDF methods to discretizate the time derivative term in (5.2) yield the following systems:

$$\left(\frac{1}{\Delta t}M + K\right)\Phi^{i+1} = F^{i+1} + \frac{1}{\Delta t}M\Phi^{i}, \tag{5.3}$$

$$\left(\frac{1}{\Delta t}M + \frac{2}{3}K\right)\Phi^{i+1} = \frac{2}{3}F^{i+1} + \frac{1}{\Delta t}M\left(\frac{4}{3}\Phi^{i} - \frac{1}{3}\Phi^{i-1}\right), \tag{5.4}$$

$$\left(\frac{1}{\Delta t}M + \frac{6}{11}K\right)\Phi^{i+1} = \frac{6}{11}F^{i+1} + \frac{1}{\Delta t}M\left(\frac{18}{11}\Phi^{i} - \frac{9}{11}\Phi^{i-1} + \frac{2}{11}\Phi^{i-2}\right), \tag{5.5}$$

where Δt is the time step and Φ^i is the solution at time step i. Similarly, F^i is the value of F at time step i.

All the BDF methods are implicit in time and stable. The accuracies of the methods increase along with the increasing order. The starting values for the BDF schemes of order $n > 1$ are computed using the BDF schemes of order $1, ..., n-1$ as starting procedures. It should be noted that the BDF discretizations of order $n > 3$ do not allow the use of variable time-step size. Adaptive time-stepping strategy may also be used in the case of the first order BDF scheme.

The adaptive time-stepping is accomplished by first solving the system using a trial time step and then using two time steps the lengths of which equal to the half of that of the trial time step and comparing the results. If the difference between the results is found to be sufficiently small, the use of the trial time step is accepted. Otherwise a new trial time step is defined by dividing the previous trial time step into two steps of equal length and then the procedure is repeated. One may define one's own criterion for determining whether the use of the current time step is accepted. The default criterion is that the norms of the solutions to each system of field equations do not differ more than the given threshold value.

The time discretization of the second order equation

$$M\frac{\partial^2\Phi}{\partial t^2} + B\frac{\partial\Phi}{\partial t} + K\Phi = F \tag{5.6}$$

using the Bossak method leads to the system

$$\begin{aligned}\left(\frac{1-\alpha}{\beta(\Delta t)^2}M + \frac{\gamma}{\beta\Delta t}B + K\right)\Phi^{i+1} = F^{i+1} + M\left(\frac{1-\alpha}{\beta(\Delta t)^2}\Phi^i + \frac{\gamma}{\beta\Delta t}V^i + \frac{(1-\alpha)}{2\beta}A^i\right) + \\ B\left(\frac{\gamma}{\beta\Delta t}\Phi^i + \left(\frac{\gamma}{\beta}-1\right)V^i + \left(1-\frac{\gamma}{2\beta}\right)\Delta t A^i\right),\end{aligned} \tag{5.7}$$

where

$$\begin{aligned}V^{i+1} &= V^i + \Delta t\left((1-\gamma)A^i + \gamma A^{i+1}\right),\\ A^{i+1} &= \frac{1}{\beta(\Delta t)^2}(\Phi^{i+1}-\Phi^i) - \frac{1}{\beta\Delta t}V^i + \left(1-\frac{1}{2\beta}\right)A^i,\\ \beta &= \frac{1}{4}(1-\alpha)^2, \quad \gamma = \frac{1}{2}-\alpha.\end{aligned} \tag{5.8}$$

In the following the matrices M and B are referred to as the mass and damping matrix, respectively.

5.3 Keywords related to time discretization

All the keywords related to the time discretization may be given in Simulation section of the solver input file (.sif file). A number of keywords may also be given in Solver section, so that each system of field equations may be discretizated using independently chosen time-stepping method. If keywords are not given in the Solver section, the values of the keywords are taken to be those given in the Simulation section. It should be noted that certain keywords such as those controlling the number of time steps, time-step sizes etc. may only be given in the Simulation section.

`Timestepping Method` `String`

This keyword is used to declare the time discretization strategy for the first order equations. The value of this keyword may be set to be either `"BDF"` or `"Crank-Nicolson"` and may be given in either Simulation section or Solver section of the solver input file.

`BDF Order` `Integer`

This keyword is used to define the order of the BDF method and may take values 1,...,5. This keyword may be given in either Simulation section or Solver section of the solver input file.

`Time Derivative Order` `Integer`

If a second order equation is discretizated, this keyword must be given the value 2 in the Solver section of the solver input file. It should be noted that the second order time derivatives are always discretizated using the Bossak method.

`Bossak Alpha` `Real [-0.05]`

This keyword is used to define the value for α in the Bossak method used in the time discretization of second order equations. This keyword may be given in either Simulation section or Solver section of the solver input file.

`Timestep Intervals` `Integer array`

This keyword is used to define the number of time steps. It may be array-valued so that different time-step lengths may be used for different time intervals of the entire simulation. For example, if one wishes to take first 50 time steps and then to use a different time-step length for the following 100 time steps, one may define

```
Timestep Intervals(2) = 50 100
```

and use the `Timestep Sizes` keyword to define time-step lengths for the two sets of time steps.

`Timestep Sizes` `Real array`

This keyword is used to define the length of time step. If the value of the `Timestep Intervals` keyword is array-valued, the value of this keyword must also be an array of the same size. For example, if one has defined

```
Timestep Intervals(2) = 50 100
```

the declaration

```
Timestep Sizes(2) = 0.1 1.0
```

sets the time-step length for the first 50 time steps to be 0.1 and for the remaining 100 time steps 1.0.

`Timestep Function` `Real`

Instead of using the `Timestep Sizes` keyword the length of time step may be defined by using this keyword. The value of this keyword is evaluated at the beginning of each time step. A variable time-step length may conveniently be defined using a MATC or Fortran function.

`Output Intervals` `Integer array`

This keyword is used to define the time-step interval for writing the results on disk. As in the case of the `Timestep Sizes` keyword the size of the value of this keyword must be compatible with that of the `Timestep Intervals` keyword. The value at a step m is saved if for the corresponding output interval o `mod(m-1,o)==0`. An exception is output interval equal to zero for which output is not saved at all. However, the last step of the simulation is always saved.

`Lumped Mass Matrix` `Logical [false]`

The use of a lumped mass matrix may be activated by setting the value of this keyword to be `True` in the Solver section of solver input file. The default lumping is defined by

$$M'_{ii} = M_{ii} \frac{\sum_i \sum_j M_{ij}}{\sum_i M_{ii}}. \tag{5.9}$$

The keywords related to the adaptive time-stepping may only be given in the Simulation section of the solver input file. When the adaptive time-stepping strategy is used, a set of trial time steps is defined using the keywords introduced above. The adaptive procedure is executed for each of these trial steps. Note that the adaptive time-stepping is possible only in the case of the first order BDF scheme.

`Adaptive Timestepping` `Logical [false]`

The value of this keyword must be set to be `True` if the adaptive time integration is to be used.

`Adaptive Time Error` `Real`

This keyword is used to define the threshold value for the criterion for determining whether the use of the current time step is accepted.

`Adaptive Error Measure` Real

Using this keyword one may define one's own measure for evaluating the difference between the computed results. This measure and the threshold value, which is given using the `Adaptive Time Error` keyword, may be used to define a user-defined criterion for determining whether the use of the current time step is accepted. The value of the `Adaptive Error Measure` keyword is evaluated twice for each trial time step. For the first time the value of the keyword is evaluated after the system is solved using the trial time step. The second time is after the system is solved using two time steps the lengths of which equal to the half of that of the trial time step. The absolute value of the relative difference between these two values is compared to the threshold value given by the `Adaptive Time Error` keyword to determine whether the use of the current time step is accepted. If several systems of field equations are solved, all the solutions must satisfy the similar criterion. If this keyword is not used, the default criterion is based on comparing the norms of the solution fields.

`Adaptive Min Timestep` Real

Using this keyword one can limit the subsequent division of the trial time steps by giving the minimum time-step length which is allowed.

`Adaptive Keep Smallest` Integer [1]

By default the adaptive scheme tries to double the length of the time step after the acceptable time step is found. If a value $n > 1$ is given for this keyword, the adaptive scheme tries to increase the step length after taking n steps which are at most as long as the step length accepted.

5.4 On the treatment of time derivatives in Elmer Solver code

In the following a number of issues that may be useful if one is writing a code to solve one's own application are explained.

By default Elmer Solver does not generate or use global mass or damping matrices in the solution of time-dependent systems. Mass and damping matrices need to be computed only element-wise, as the linear system resulting from the time discretization, such as (5.3), is first formed element-wise and this local contribution is later assembled to the global system. In the case of the first order equation (5.2) the local linear system may be formed by using the subroutine call

```
CALL Default1stOrderTime( M, K, F ),
```

where M is the element mass matrix, K is the element stiffness matrix and F is the element force vector. In a similar manner, in the case of the second order equation (5.6) one may use the subroutine call

```
CALL Default2ndOrderTime( M, B, K, F ),
```

where B is the element damping matrix.

Note that these subroutines must also be called for the local matrices and vectors that result from the discretization of neumann and newton boundary conditions. If the boundary conditions do not contain any time derivatives, the M and B matrices should be set to be zero before calling the above subroutines.

If the global mass matrix is required, it may be generated by using the subroutine call

```
CALL DefaultUpdateMass( M )
```

Similarly, the global damping matrix may be generated by using the subroutine call

```
CALL DefaultUpdateDamp( B ).
```

Global mass (and possibly damping) matrices are required, for example, in the solution of eigenvalue problems. One may also implement one's own time-stepping scheme at the global level using these matrices.

Chapter 6

Solving eigenvalue problems

6.1 Introduction

Eigenvalue problems form an important class of numerical problems, especially in the field of structural analysis. Also some other application fields may have eigenvalue problems, such as those in density functional theory. This manual, however, introduces eigenvalue computation in Elmer using terminology from elasticity.

Several different eigenvalue problems can be formulated in elasticity. These include the "standard" generalized eigenvalue problems, problems with geometric stiffness or with damping, as well as stability (buckling) analysis. All of the aforementioned problems can be solved with Elmer. The eigenproblems can be solved using direct, iterative or multigrid solution methods.

6.2 Theory

The steady-state equation for elastic deformation of solids may be written as

$$-\nabla \cdot \tau = \vec{f}, \tag{6.1}$$

where τ is the stress tensor. When considering eigen frequency analysis, the force term $\vec{f}$ is replaced by the inertia term,

$$-\nabla \cdot \tau = \rho \frac{\partial^2 \vec{d}}{\partial t^2}, \tag{6.2}$$

where ρ is the density.

The displacement can now be assumed to oscillate harmonically with the eigen frequency ω in a form defined by the eigenvector $\vec{d}$. Inserting this into the above equation yields

$$-\nabla \cdot \tau(\vec{d}) = -\omega^2 \rho \vec{d}, \tag{6.3}$$

or in discretized form

$$Ku = -\omega^2 M u, \tag{6.4}$$

where K is the stiffness matrix, M is the mass matrix, and u is a vector containing the values of $\vec{d}$ at discretization points. The equation 6.4 is called the generalized eigenproblem.

Including the effects of pre-stresses into the eigenproblem is quite straightforward. Let us assume that there is a given tension field σ in the solid. The tension is included by an extra term in the steady-state equation

$$-\nabla \cdot \tau - \nabla \cdot (\sigma \nabla u) = \vec{f}. \tag{6.5}$$

The pre-stress term includes a component K_G to the stiffness matrix of the problem and thus the eigenvalue equation including pre-stresses is

$$(K + K_G)u = -\omega^2 M u. \tag{6.6}$$

The pre-stress in Elmer may be a known pre-tension, due to external loading or due to thermal stress, for example. The stress tensor containing the pre-stresses σ is first computed by a steady-state analysis and after that the eigenvalue problem is solved. It should be noted though that the eigenvalue problem in a pre-stressed state is solved using first order linearization, which means that the eigenvalues are solved about the non-displaced state. If the pre-loading influences large deformations the eigenvalues are not accurate.

The eigenvalue problem with pre-stresses may be used to study the stability of the system. Some initial loading is defined and a pre-stress tensor σ is computed. This tensor is then multiplied by a test scalar λ. The critical load for stability, or buckling, is found by setting the force on the right hand side of the equation 6.5 equal to zero. The problem then is to solve λ from

$$Ku = -\lambda K_G u, \tag{6.7}$$

which again is formally an eigenvalue problem for the test parameter. The critical loading is found by multiplying the given test load with the value of λ. In other words, if $\lambda > 1$ the loading is unstable.

6.2.1 Damped eigenvalue problem

Finally, let us consider the damped eigenproblem, also called quadratic eigenvalue problem. In this case there is a force component proportional to the first time derivative of the displacement in addition to the inertia term

$$-\nabla \cdot \tau = -\delta \frac{\partial \vec{d}}{\partial t} + \rho \frac{\partial^2 \vec{d}}{\partial t^2}, \tag{6.8}$$

where δ is a damping coefficient. The problem is transformed into a more suitable form for numerical solution by using a new variable $\vec{v}'$ defined as $\vec{v}' = \frac{\partial \vec{d}}{\partial t}$. This yields

$$-\nabla \cdot \tau = -\delta \vec{v}' + \rho \frac{\partial \vec{v}'}{\partial t}. \tag{6.9}$$

Working out the time derivatives and moving into the matrix form, the equation may be written as

$$Ku = -Dv + i\omega M v, \tag{6.10}$$

or,

$$-i\omega \begin{pmatrix} I & 0 \\ 0 & M \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 & I \\ -K & -D \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}, \tag{6.11}$$

where i is the imaginary unit, D is the damping matrix, and v a vector containing the values of $\vec{v}'$ at the discretization points. Now the damped eigenproblem is transformed into a generalized eigenproblem for complex eigenvalues.

Finally, to improve the numerical behavior of the damped eigenproblem, a scaling constant s is introduced into the definition $s\vec{v}' = s\frac{\partial \vec{d}}{\partial t}$. In the matrix equation 6.11 this influences only the identity matrix blocks I to be replaced by sI. Good results for numerical calculations are found when

$$s = ||M||_\infty = \max |M_{i,j}|. \tag{6.12}$$

6.3 Keywords related to eigenvalue problems

An eigenvalue analysis in Elmer is set up just as the corresponding steady-state elasticity analysis. An eigenvalue analysis is then defined by a few additional keywords in the Solver section of the sif file. The solver in question can be linear elasticity solver called Stress Analysis, linear plate elasticity solver, or even nonlinear elasticity solver, though the eigen analysis is, of course, linear.

Many of the standard equation solver keywords affect also the eigen analysis, *e.g.* the values given for Linear System Solver and Linear System Iterative Method in case of an iterative solver. More information about these settings is given in this Manual under the chapter concerning linear system solvers. The specific keywords for eigen analysis are listed below

`Eigen Analysis` Logical
: Instructs Elmer to use eigensystem solvers. Must be set to True in all eigenvalue problems.

`Eigen System Values` Integer
: Determines the number of eigen values and eigen vectors computed.

`Eigen System Select` String
: This keyword allows the user to select, which eigenvalues are computed. The allowable choices are

- Smallest Magnitude
- Largest Magnitude
- Smallest Real Part
- Largest Real Part
- Smallest Imag Part
- Largest Imag Part

Smallest magnitude is the default.

`Eigen System Convergence Tolerance` Real
: The convergence tolerance for iterative eigensystem solver. The default is 100 times Linear System Convergence Tolerance.

`Eigen System Max Iterations` Integer
: The number of iterations for iterative eigensystem solver. The default is 300.

`Eigen System Complex` Logical
: Should be given value True if the eigen system is complex, *i.e.* the system matrices are complex. Not to be given in damped eigen value analysis.

`Geometric Stiffness` Logical
: Defines geometric stiffness (pre-stress) to be taken into account in eigen analysis. This feature is only available with linear bulk elasticity solver.

`Stability Analysis` Logical
: Defines stability analysis. This feature is only available with linear bulk elasticity solver.

`Eigen System Damped` Logical
: Defines a damped eigen analysis. Damped eigen analysis is available only when using iterative solver.

`Eigen System Use Identity` Logical
: If True defines the relation displacement and its derivative to be $s\vec{v}' = s\frac{\partial \vec{d}}{\partial t}$. The other possibility is to use $Mv = i\omega Mu$. The default is True.

6.4 Constructing matrices M and D in Solver code

In eigen analysis the mass matrix M and the damping matrix D have to be separately constructed. Usually in Elmer the different matrices are summed into a single matrix structure, since the final linear equation is of the form $Ax = b$, and there is no need for separate values of the mass matrix and the stiffness matrix.

The matrix is represented in Elmer using compressed row storage (CRS) format, as explained in chapter about Linear system solvers. The matrix structure holds also vectors for the values of the mass and damping matrices

```
TYPE Matrix_t
   ...
  REAL(KIND=dp),  POINTER :: MassValues(:), DampValues(:)
   ...
END TYPE Matrix_t
```

These arrays use the same `Rows` and `Cols` tables than the normal `Values` array.

The mass and damping matrices are constructed elementwise in a similar manner as the stiffness matrix. After each element the local contributions are updated to the equation matrices by the following subroutine calls

```
CALL DefaultUpdateEquations( STIFF, FORCE )

IF ( Solver % NOFEigenValues > 0 ) THEN
  CALL DefaultUpdateMass( MASS )
  CALL DefaultUpdateDamp( DAMP )
END IF
```

In this segment of code the variables `STIFF`, `MASS`, `DAMP` and `FORCE` store the local values of the stiffness matrix, the mass matrix, the damping matrix, and the right hand side of the equation, respectively. The integer `NOFEigenValues` if the `Solver` data structure gives the number of eigen values requested. Here it is used as an indicator of whether the mass and damping matrices need to be constructed.

The eigenvalues and eigenvectors are stored in the arrays `Solver % Variable % EigenValues` and `Solver % Variable % EigenVectors`,

```
TYPE Variable_t
   ...
  COMPLEX(KIND=dp), POINTER :: EigenValues(:)
  COMPLEX(KIND=dp), POINTER :: EigenVectors(:,:)
   ...
END TYPE Matrix_t
```

and the eigenvector corresponding to the eigenvalue `i` is found in `Solver % Variable % EigenVectors(i,:)`.

Chapter 7

Adaptive Solution

7.1 Introduction

A posteriori error analysis and adaptive mesh refinement are nowadays standard tools in finite element analysis when cracks, boundary layers, corner singularities, shock waves, and other irregularities are present. A posteriori error indicators can be used to reveal flaws in finite element discretizations and well designed adaptive mesh refinemenets can reduce the computational costs drastically.

7.2 Theory

Let us consider equilibrium equations of the form

$$-\nabla \cdot q = f \ \text{ in } \Omega, \tag{7.1}$$

$$q \cdot n = g \ \text{ on } \Gamma, \tag{7.2}$$

where q is either a flux vector or a second order stress tensor, Ω is a computational domain, Γ is a boundary part, f is an external source or body force, g is an external flux or traction and n is the unit outward normal to the boundary.

Most symmetric steady state problems described in the model manual of Elmer [] fit in the above framework of equilibrium equations. To fix ideas, suppose that q is the heat flux satisfying Fourier's law $q = -k\nabla T$, where T is the temperature and k is the heat conductivity of the material. We could also think of q as the stress tensor of linear elasticity. In this case Hooke's law states that $q = \mathcal{E} : \varepsilon$, where $\mathcal{E}$ is the fourth order tensor of elastic coefficients, $\varepsilon = symm(\nabla u)$ is the linearized strain tensor and u is the displacement vector.

7.2.1 A posteriori estimate

Let us denote the finite element approximation of q by q_h and measure the error $q - q_h$ as

$$ERROR = \sqrt{\int_\Omega |q - q_h|^2 \, d\Omega} \tag{7.3}$$

Our primary goal is to ensure the accuracy of the solution by imposing the condition

$$ERROR \leq TOLERANCE \tag{7.4}$$

where $TOLERANCE > 0$ is an error tolerance prescribed by the user.

In practise, the goal must be replaced by a stronger condition

$$ESTIMATE \leq TOLERANCE \tag{7.5}$$

where $ESTIMATE$ is a computable functional (of all available data) satisfying

$$ERROR \leq ESTIMATE \tag{7.6}$$

Then, if (7.5) holds, (7.4) is satisfied and the quality of the numerical solution is guaranteed.

In Elmer the a posteriori estimate (7.5) is computed from local residuals of the finite element solution as a weighted sum over the elements,

$$ESTIMATE = \sqrt{\sum_E \eta_E^2}, \tag{7.7}$$

where η_E is the local error indicator for an individual element E:

$$\begin{aligned} \eta_E^2 &= \alpha_E h_E^2 \int_E \left|\nabla \cdot q_h + f\right|^2 d\Omega \\ &+ \quad \beta_E \sum_{e\ in\ \Omega} h_e \int_e \left|[\![q_h \cdot n_e]\!]_e\right|^2 d\Gamma \\ &+ \quad \gamma_E \sum_{e\ on\ \Gamma} h_e \int_e \left|q_h \cdot n_e - g\right|^2 d\Gamma \end{aligned} \tag{7.8}$$

Here α_E, β_E, and γ_E, are local positive constants. The values of these constants depend, among other things, on the problem to be solved, and must be estimated carefully case by case [].

The first sum in (7.8) is taken over all edges e of E inside the computational domain, the second sum is taken over all edges on the boundary part Γ, $[\![\cdot]\!]_e$ is the jump in $(\cdot)$ across e, and n_e is a unit normal to the edge. h_E is the size of the element and h_e is the size of the edge.

The first term on the right-hand-side of (7.8) measures the local residual of the finite element solution with respect to the equilibrium equation (7.1). The second term measures the discontinuity in the numerical flux inside Ω and the third term the residual with respect to the boundray condition (7.2).

7.2.2 Adaptivity

The secondary goal of our numerical computations is to find a solution satisfying (7.4) as efficienciently as possible. A nearly optimal solution strategy is obtained by utilizing the property (here we need to impose some minor restrictions on f and g, see [])

$$LOCAL\ ERROR \geq \eta_E \tag{7.9}$$

where

$$LOCAL\ ERROR = \sqrt{\int_E |q - q_h|^2\, d\Omega} \tag{7.10}$$

The estimate suggests that the error in the numerical solution should be reduced efficiently if the mesh is refined locally where the indicators η_E are large. Naturally, we can think of coarsening the mesh where the values of the indicators are small.

The adaptive mesh refinement strategy of Elmer is based on the local estimate (7.9) and on the following additional assumptions and heuristic optimality conditions:

- The local error behaves as

  $$\eta_E = C_E h_E^{p_E} \tag{7.11}$$

  for some constants C_E and p_E.

- In the optimal mesh the error is uniformly distributed over the elements:

  $$\eta_E = TOLERANCE/N_{elements} \tag{7.12}$$

The constants C_E and p_E in (7.11) can be solved locally for each element if the local errors and the local mesh sizes are known from at least two different solutions. The second rule (7.12) can then be applied to extrapolate a new nearly optimal mesh density for the subsequent calculations.

The mesh refinements can be performed eiher by splitting the existing elements into smaller using the so called RGB-refinement strategy described in [], or by permorming a complete remeshing of the computational domain using the built-in unstructured mesh generators that produce high quality Delaunay triangulations. In the latter alternative not only mesh refinement is possible, but also local adaptive coarsening.

7.3 Keywords related to the adaptive solution

The adaptive solver of Elmer is activated and controlled by the following keywords in the Solver block of the solver-input-file.

`Adaptive Mesh Refinement` `Logical`
: If set to true, then after the solution of the linear system the program computes residual error indicators for all active elements, estimates the global error, computes a new mesh density and refines the mesh accordingly.

`Adaptive Remesh` `Logical`
: If set to true, then a complete remeshing is performed after error estimation using the Mesh2D or Mesh3D generators. The new mesh density is written in file “bgmesh”. If set to false, then the RGB-splitting strategy for triangles is applied to perform the refinements.

`Adaptive Save Mesh` `Logical`
: If set to true, the subsequent meshes are stored in directories `RefinedMeshN`, where `N` is the number of the adaptive iterate.

`Adaptive Error Limit` `Real`
: Error tolerance for the adaptive solution.

`Adaptive Min H` `Real`
: Imposes a restriction on the mesh size. Defualt is zero.

`Adaptive Max H` `Real`
: Imposes a restriction on the mesh size. Default is infinite.

`Adaptive Max Change` `Real`
: Controls the change in local mesh density between two subsequent adaptive iterates. Using this keyword the user can restrict the refinement/coarsening to stabilize the adaptive solution process.

7.4 Implementing own error estimators

Suppose that we are given a subroutine called `MySolver` for solving the Poisson equation, and we would like to enhance the code by implementing an a posteriori error indicator for adaptive mesh refinement. The first thing to do is to take the module `Adaptive` in use, an define the local error indicators as functions in an intefrace block. The beginning of the subroutine should look like the following:

```
SUBROUTINE MySolver( Model,Solver,Timestep,TransientSimulation )
  USE DefUtils
  USE Adaptive

  INTERFACE
    FUNCTION InsideResidual( Model, Element, Mesh, &
        Quant, Perm, Fnorm ) RESULT( Indicator )
      USE Types
      TYPE(Element_t), POINTER :: Element
      TYPE(Model_t) :: Model
      TYPE(Mesh_t), POINTER :: Mesh
      REAL(KIND=dp) :: Quant(:), Indicator, Fnorm
      INTEGER :: Perm(:)
    END FUNCTION InsideResidual

    FUNCTION EdgeResidual( Model, Edge, Mesh, &
        Quant, Perm ) RESULT( Indicator )
      USE Types
      TYPE(Element_t), POINTER :: Edge
      TYPE(Model_t) :: Model
      TYPE(Mesh_t), POINTER :: Mesh
      REAL(KIND=dp) :: Quant(:), Indicator
      INTEGER :: Perm(:)
    END FUNCTION EdgeResidual

    FUNCTION BoundaryResidual( Model, Edge, Mesh, &
        Quant, Perm, Gnorm ) RESULT( Indicator )
      USE Types
      TYPE(Element_t), POINTER :: Edge
      TYPE(Model_t) :: Model
      TYPE(Mesh_t), POINTER :: Mesh
      REAL(KIND=dp) :: Quant(:), Indicator, Gnorm
      INTEGER :: Perm(:)
    END FUNCTION BoundaryResidual
  END INTERFACE
```

After these fixed declarations we may proceed normally by defining the local variables, allocate memory for local tables, integrate the stiffness matrix, set boundary conditions, and solve the problem. Error estimation and adaptive mesh refinements are then performed by calling the subroutine `RefineMesh`, which should appear in the code right after the function `DefaultSolve`.

```
  Norm = DefaultSolve()

  IF ( ListGetLogical( Solver % Values, 'Adaptive Mesh Refinement' ) ) &
      CALL RefineMesh( Model, Solver, Potential, Permutation, &
              InsideResidual, EdgeResidual, BoundaryResidual )
```

The functions `InsideResidual`, `EdgeResidual` and `BoundaryResidual` defined in the interface block should finally be contained in `MySolve`, and return the values of the error indicators described in the previous section.

As an example, suppose that we are using linear triangles or tetrahedra for solving the Poisson equation. In this case it holds $\nabla \cdot q_h = 0$ on each element E, and the contribution of the firtst term in (7.1) is simply

$$\texttt{InsideResidual} = h_E \sqrt{\int_E |f|^2 \, d\Omega} \tag{7.13}$$

The function that computes the value of the inside redisual could be written as follows.

```
FUNCTION InsideResidual( Model, Element, Mesh, &
        Quant, Perm, Fnorm ) RESULT( Indicator )
  IMPLICIT NONE
  TYPE(Model_t) :: Model
  INTEGER :: Perm(:)
  REAL(KIND=dp) :: Quant(:), Indicator, Fnorm
  TYPE( Mesh_t ), POINTER    :: Mesh
  TYPE( Element_t ), POINTER :: Element

  TYPE(GaussIntegrationPoints_t), TARGET :: IP
  TYPE(ValueList_t), POINTER :: BodyForce
  REAL(KIND=dp) :: f, hK, detJ, Basis(MAX_NODES), &
    dBasisdx(MAX_NODES,3), ddBasisddx(MAX_NODES,3,3), &
    Source(MAX_NODES)
  LOGICAL :: stat
  INTEGER :: n

  Indicator = 0.0d0
  Fnorm = 0.0d0
  hK = element % hK

  BodyForce => GetBodyForce( Element )
  Source = GetReal( Element, 'Source' )

  IP = GaussPoints( Element )
  DO n = 1, IP % n
    stat = ElementInfo( Element, Nodes, IP % u(n), IP % v(n), &
        IP % w(n), detJ, Basis, dBasisdx, ddBasisddx, .FALSE. )
    f = SUM( Source * Basis )
    Fnorm = Fnorm + f**2 * detJ % IP % s(n)
    Indicator = Indicator + f**2 * detJ * IP % s(n)
  END DO

  Fnorm = SQRT( Fnorm )
  Indicator = hK * SQRT( Indicator )

END FUNCTION Inside Residual
```

For the boundary and edge residuals refer to the example `Poisson.f90` in the tutorial manual of Elmer.

Chapter 8

Matrix manipulation utilities

8.1 Dirichlet conditions

In finite element method there are two kinds of boundary conditions. The natural boundary condition that may be set by only affecting the r.h.s. of the equation and the essential boundary conditions where also the matrix needs to be tampered. The latter ones are also called Dirichlet boundary conditions. The natural boundary conditions are often more problem specific so the user is directed to the Models Manual for more details on them.

Technically the Dirichlet conditions in ElmerSolver are set through manipulating only the values in the matrix rather than its structure. To be more specific, in setting the degree of freedom with index i the i:th row of the matrix is set zero, except for the diagonal which is set to be unity. When also the r.h.s. of the equation is set to the desired value, the solution will satisfy the Dirichlet condition. The Dirichlet conditions may be set to existing boundary elements. Additionally Dirichlet conditions may be set for set of nodes that are created on-the-fly.

Usually the Dirichlet conditions are given at objects which have a lower dimension than the leading dimension in the geometry, i.e. for 3D problems values are usually fixed only at 2D faces. However, it is possible also to set the conditions for the bodies also. This may be particularly useful when the condition is only conditional.

There is a handicap with this procedure which is that the symmetry of the original matrix will be lost. This may affect the performance of linear system solvers. To ensure to symmetricity of the matrix equation there are two remedies. Also the column may be zeroed and the known values may be subtracted from the r.h.s. The second option is to eliminate all the rows and columns related to the known values. This reduces the size of the matrix but of has an additional cost as a secondary matrix is created and the values are copied into it.

Sometimes the Dirichlet conditions should depend on other variables in a way which defined whether or not to set the conditions at all. For example, the temperature at a boundary should be defined only if the flow is inside the boundary. For outflow the definition of the temperature is not physically justified. For this kind of purposes the user may give a condition that is a variable in itself. If this variable is positive the Dirichlet condition is applied,

8.2 Periodic conditions

Periodic BCs may be considered to be a special case of Dirichlet conditions where the fixed value is given as linear combination of other unknown values. The periodic boundary conditions in Elmer are very flexible. In fact they may even be antiperiodic.

8.3 Setting and computing nodal loads

Similarly to the Dirichlet values one may also set nodal loads i.e. entries for the r.h.s. of the matrix equation. Generally there are good reasons to avoid the use of nodal loads as they are mesh dependent. There are, however, some uses also for setting nodal loads. For example, in multiphysical couplings sometimes it may be a good solution to transfer the forces directly in nodal form as this is the most accurate way to compute the forces resulting from the discrete system.

It is possible to evaluate the nodal loads after the solution is computed. This however, requires that the original matrix A_0 that has not been eliminated for Dirichlet conditions is saved. Then the the nodal forces may be computed from

$$f = A_0 x - b. \tag{8.1}$$

It should be noted that the nodal value is mesh dependent. For heat equation it will be in Watts and for electrostatic equation in Coulombs, for example.

8.4 Active and passive elements

In Elmer it is possible to define certain areas of the modeled geometry passive during the solution. This feature allows also deactivating and reactivating of the elements. An element being passive means that its contribution is not included into the global matrix equation. One could, for example, model two separate bodies heated with different heating power, and connect them with a third structure only after suitable time has elapsed. This all could be modeled within a single simulation.

The geometry of the whole system is meshed as usual, and the passive elements are only omitted from the equations. The passive definition is done solverwise and elementwise. The former means that, eg., the temperature may be passive and the displacements active at the same element. The passive property of elements is defined with a real valued parameter with the name constructed from the name of the variable followed by `Passive` in the `Body Force` section. When the parameter obtains a value greater than zero the element is passive.

8.5 Keywords for Matrix manipulation

`Solver` `solver id`

`Linear System Symmetric` `Logical True`
: Make the matrix symmetric by eliminating the known values from the r.h.s and zeroing the matrix entries.

`Before Linsolve` `"EliminateDirichlet" "EliminateDirichlet"`
: Creates a secondary matrix with a reduced size by eliminating Dirichlet conditions and passing this to the linear system solver.

`Calculate Loads` `Logical True`
: This keyword activates the computation of nodal loads. The resulting values will be saved to variable which is derived from the primary variable by adding the suffix `Loads` to it.

`Exported Variable i` `Varname Loads`
: One may reserve the space for the load variable also explicitely by using this keyword. This may be needed if there is a dependency between variables that is needed before the load variable is created.

`Boundary Condition` `bc id`

`Target Boundaries(n)` `Integer`
: The set of boundaries for which the Dirichlet conditions will be applied on.

`Target Nodes(n)` `Integer`
: Sets point conditions on-the-fly. These points refer to the obsolute indexing of the nodes.

`Target Coordinates(n,DIM)` `Real`
: Ccoordinate values which are transformed into nodal indexes corresponding to the nearest nodes at the time of first call. Target groups defined by `Target Boundaries`, `Target Nodes`, and `Target Coordinates` should not reside in the same boundary condition definition.

`Varname` `Real`
: Each variable which has an equation that is solved for, may be set by giving its value at the boundary conditions section. If the variables are not listed in the keyword listing the user shoul also define the type which is `Real`.

`Varname i` `Real`
: For multicomponent fields the Dirichlet condition may be set to each field separately.

`Varname Condition` `Real`
: The Dirichlet condition related to the variable is set active only if the condition is positive.

`Varname Load` `Real`
: Sets the goven value to the r.h.s. of the matrix equation related to the solution of the variable. Note that this value is a nodal quantity. The nodal loads are given exactly as the Dirichlet conditions except that a string `Load` is attached to the name of the variable.

The following keywords in the boundary condition section are used to control the periodic boundary conditions.

`Periodic BC` `Integer`
: This refers to the counterpart of the periodic boundary condition. This means that periodic boundaries come in pairs, and for the other boundary you only need to give pointer to.

`Anti Periodic BC` `Integer`
: The system may be also antiperiodic i.e. the absolute value is the same but the sign is different.

`Periodic BC Translate(3)` `Real`
: The periodic boundary is mapped to the other boundary by three different operations: translation, rotatition and scaling. This generality is not usually needed and therefore default value is used. For the translation vector the default is the vector that is obtained when moving in the normal direction of the first boundary until the target boundary is hit. If this is not desired the user may give another translation vector using this keyword.

`Periodic BC Rotate(3)` `Real`
: By default no rotation is performed prior to the mapping of values. This keyword may be used to give the angles of rotation.

`Periodic BC Scale(3)` `Real`
: By default there is no scaling performed prior to the mapping of values. This keyword may be used to give a scaling vector if this is desired.

`Periodic BC Variable` `Logical True`
: The user should define the variables that are to be periodic in nature. This is done by attaching their names into logical expressions following the string `Periodic BC`.

`Body Force` `body force id`

`Varname` `Real`
: The setting of Dirichlet conditions for the whole body follows the same logic as for the boundaries. When the body force is assigned to a body the values will be fixed as defined.

`Varname Load` `Real`
: Sets the goven value to the r.h.s. of the matrix equation related to the solution of the variable. Note that this value is a nodal quantity. The nodal loads are given exactly as the Dirichlet conditions except that a string `Load` is attached to the name of the variable.

`Varname Passive` `Real`
: If this variable obtains a positive value the element is set passive and assembled for. Note that it is not possible to control components of vector valued variables separately.

Chapter 9

Miscallenous options

9.1 Solver activation

There is a large number of different ways how solvers need to be activated and deactivated. Mostly there needs are related to different kinds of multiphysical coupling schemes. In the solver section one may give the following keywords.

`Exec Solver` String
: The options are `never, always, before timestep, after timestep, bofore all, after all, before saving, after saving`. If nothing else is specified the solver is called every time in its order of appearance. The saving instance refers to the one defined by `Output Intervals` and used to save the results.

`Exec Interval` Integer
: This keyword gives an interval at which the solver is active. At other intervals the solver is not used.

9.2 Options for variable names

Sometimes one wants to give rename the components of the primary variable. This may be done in defining the component names in the brackets, for example.

```
Variable = Flow[Velo:2 Pres:1]
```

Decleares that variable `Flow` consists of `Velo` with two components and `Pres` with one component. If the number of components is 2 or 3 the variable will be treated as a vector in the ElmerPost files.

If one does not require output for a given variable one may declear it with the `-nooutput` option e.g.

```
Variable = -nooutput Dummy
```

If one wants to decleare the number of dofs of the variable One may also use the `-dofs` option to define the number of components in a variable e.g.

```
Variable = -dofs 3 Flow
```

These different options should not be fully mixed.

Chapter 10

Compilation and Linking

10.1 Compiling the whole package

For complete up-to-date compilation instructions look at the Elmer web pages at `http:www.csc.fielmer`.

Elmer distribution comes in several different modules. Each of these may be compiled using the configure script followed by a make command. Below is a possible compilation strategy in the Unix system.

```
#!/bin/sh -f
# replace these with your compilers:
export CC=gcc
export CXX=g++
export FC=g95
export F77=g95

modules="matc umfpack mathlibs elmergrid meshgen2d eio hutiter fem"
for m in $modules; do
  cd $m ; ./configure --prefix=/opt/elmer && make && make install && cd ..
done
```

10.2 Compiling a user defined subroutine

The `elmerf90`command is provided to help compiling your own solvers, it is a wrapper script to the compiler that was used to compile the elmer that is in the `PATH`.

```
elmerf90 -o MySolver MySolver.f90
```

In the MinGW system in Windows the suffix `.dll` should preferably be used

```
elmerf90 -o MySolver.dll MySolver.f90
```

After successful compilation, the file `mysolver.dll` is to be found in the local directory. In the filename declaration of the `Procedure`-keyword in solver input file, the suffix `.dll` can be omitted

```
Solver 1
  Procedure = "mysolver" "subroutineName"
  ...
End
```

Chapter 11

Basic Programming

11.1 Introduction

The Elmer distribution contains a large set of different solvers and also the possibility to declare dependence of material properties or boundary conditions on certain variables (e.g., using the MATC language). Nevertheless, there always may occur certain physical problems that are too difficult to be handled via the solver input file. Such problems can be coped by introducing new user functions or even complete new solvers. Elmer is very flexible if certain models have to be added by the user providing her/his own code.

This chapter shall provide a brief introduction to basic programming of user functions as well as solvers that can be added to Elmer. This will be done by mainly using certain examples and explaining the programming steps occurring in these.

The Elmer Solver source is written in the programming language Fortran 90. Since the Elmer Solver binaries are compiled as shared objects, it is sufficient to just newly compile the code contributed by the user as an executable of a shared object (`.so` in UNIX and `.dll` in Windows) that dynamically is linked to the rest of the distribution. In order to provide Elmer with the needed information to be able to load an external function or solver, the following entry in the solver input file (suffix `.sif`) has to be given:

```
Procedure "filename" "procedure"
```

Where the file `filename` is the above mentioned executable that should contain the Fortran 90 subroutine or function `procedure`. The file `filename` should reside in the same directory where the solver input file is. Else, the relative or absolute path to that file should be added in front of the entry `filename`.

11.2 Basic Elmer Functions and Structures

In order to provide a better understanding for the following mainly example-based explanation some of the most often needed functions and routines provided by Elmer shall be discussed in this section. Most of these routines and functions are defined in the Fortran 90 module `DefUtils`. It has to be included in the code provided by the user giving the keyword

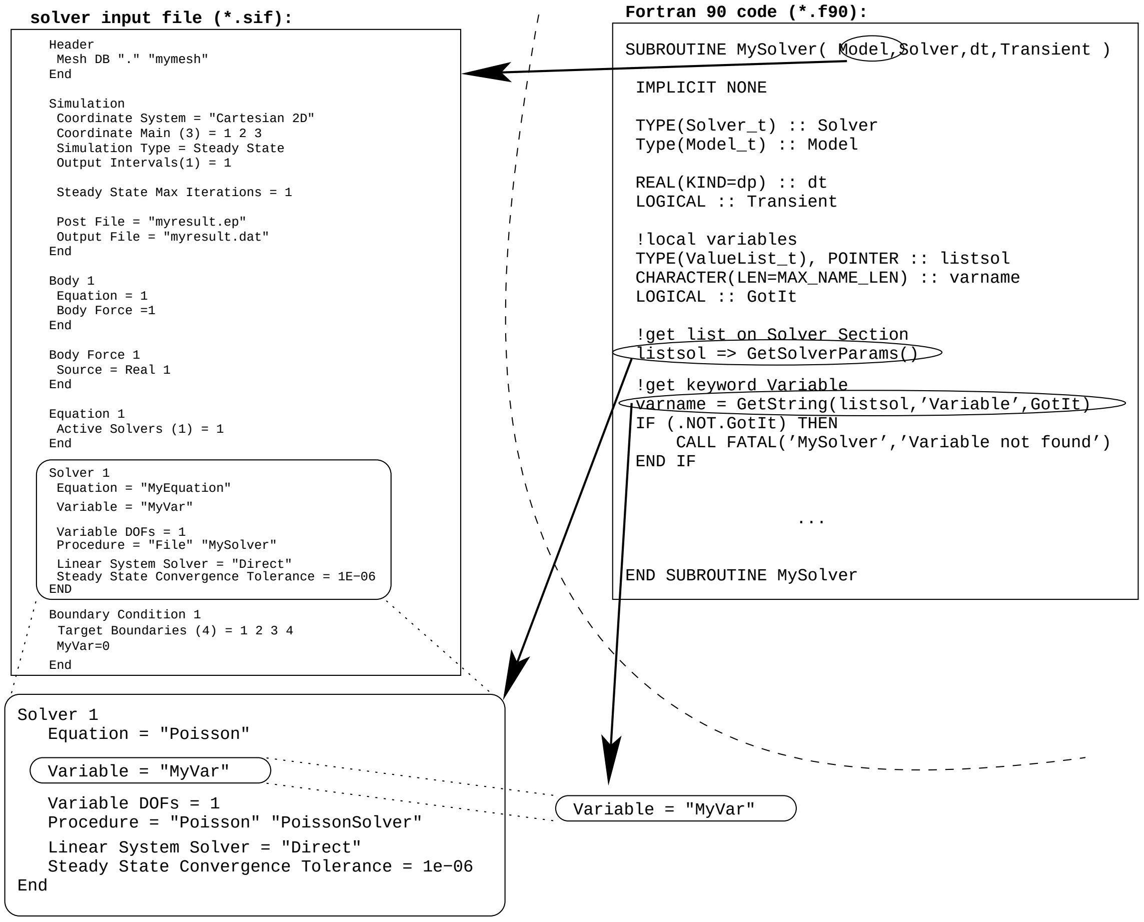
```
USE DefUtils
```

It is important to notice that – due to the nature of the Finite Element Method – the basic data structure in the Elmer Solver is the single element, rather than single points. That simplifies data manipulation in solver subroutines, but makes things a little bit more difficult if dealing with the coding of pointwise defined boundary and initial condition as well as body forces and parameter functions. In the Elmer Solver the type `Element_t` contains information on elements.

11.2.1 How to Read Values from the Input File

In the Elmer Solver the entries of each section of the solver input file – such as material, body force and initial condition – are accessed via pointer of the defined data type `ValueList_t`, further referred to as “list”. A list provides access to all the information that has been passed to the Elmer Solver from the solver input files, related to the specific section.

The principal connection between the solver input file and the access from a user function is depicted in Fig. 11.1



solver input file (*.sif):

```
Header
 Mesh DB "." "mymesh"
End

Simulation
 Coordinate System = "Cartesian 2D"
 Coordinate Main (3) = 1 2 3
 Simulation Type = Steady State
 Output Intervals(1) = 1

 Steady State Max Iterations = 1

 Post File = "myresult.ep"
 Output File = "myresult.dat"
End

Body 1
 Equation = 1
 Body Force =1
End

Body Force 1
 Source = Real 1
End

Equation 1
 Active Solvers (1) = 1
End

Solver 1
 Equation = "MyEquation"
 Variable = "MyVar"

 Variable DOFs = 1
 Procedure = "File" "MySolver"
 Linear System Solver = "Direct"
 Steady State Convergence Tolerance = 1E−06
END
Boundary Condition 1
 Target Boundaries (4) = 1 2 3 4
 MyVar=0
End
```

Fortran 90 code (*.f90):

```
SUBROUTINE MySolver( Model,Solver,dt,Transient )

 IMPLICIT NONE

 TYPE(Solver_t) :: Solver
 Type(Model_t) :: Model

 REAL(KIND=dp) :: dt
 LOGICAL :: Transient

 !local variables
 TYPE(ValueList_t), POINTER :: listsol
 CHARACTER(LEN=MAX_NAME_LEN) :: varname
 LOGICAL :: GotIt

 !get list on Solver Section
 listsol => GetSolverParams()

 !get keyword Variable
 varname = GetString(listsol,'Variable',GotIt)
 IF (.NOT.GotIt) THEN
     CALL FATAL('MySolver','Variable not found')
 END IF

                ...

END SUBROUTINE MySolver
```

```
Solver 1
   Equation = "Poisson"

   Variable = "MyVar"

   Variable DOFs = 1
   Procedure = "Poisson" "PoissonSolver"
   Linear System Solver = "Direct"
   Steady State Convergence Tolerance = 1e−06
End
```

```
Variable = "MyVar"
```

Figure 11.1: Scheme of the access of structures in the solver input file from a Fortran 90 user subroutine. The example shows, how a string is read in from the `Solver` section.

How to Access Different Sections

The following table shows the definition of the functions defined in the module `DefUtils` to provide the correct list for parameters and constants concerning the simulation and solvers

function	**corresponding section**
`GetSimulation()`	`Simulation`
`GetConstants()`	`Constants`
`GetSolverParams()`	`Solver` *`1,...`*

For instance, the following source code lines provide access to the entries in the simulation section of the solver input file

```
! variable declaration for pointer on list
TYPE(ValueList_t), POINTER :: Simulation
...
! assign pointer to list
Simulation => GetSimulation()
...
```

Lists that provide information connected to a certain element are

function	**corresponding section**
`GetMaterial( Element, Found )`	`Material` *1,...*
`GetBodyForce( Element, Found )`	`Bodyforce` *1,...*
`GetEquation( Element, Found )`	`Equation` *1,...*
`GetBC( UElement )`	`Boundary Condition` *1,...*

In the first three of these functions shown above the optional variable `Found` of type `LOGICAL` is set to `.TRUE.` upon successful search in the solver input file. Hence, it can be used for error handling. The arguments `Element` and `UElement` are of type `Element_t`. If writing a solver, the current element is known and hence can directly be passed to the functions listed above. Else, this argument may also be omitted. However, Elmer Solver needs to have the information upon the element in order to inquire the number of the material/bodyforce/equation/boundary condition section from the solver input file. Hence, if this function argument is dropped, Elmer Solver falls back to the structure `CurrentModel % CurrentElement`, which by the active solver has to be assigned to the address of the current element (see section 11.4).

The functions for input of different values from the solver input file need the assigned pointer to the corresponding to the specific section.

Reading Constants from the Solver Input File

The following value types are defined for the solver input file:

Value in Input File	**Variable in Elmer Solver**
`Real`	`Real(KIND=dp)`
`Integer`	`INTEGER`
`Logical`	`LOGICAL`
`String`	`CHARACTER(LEN=MAX_NAME_LEN)`
`File`	`CHARACTER(LEN=*)`

The defined interface of such a function is

```
FUNCTION FunctionName( List, Name, Found ) Result(x)
   TYPE(ValueList_t), POINTER :: List
   CHARACTER(LEN=*) :: Name
   LOGICAL, OPTIONAL :: Found
```

The arguments have the following purpose

`List`	List from which the value has to be read. This pointer has to be obtained by one of the previously introduced functions
`Name`	The keyword in the particular section for the value
`Found`	Optional boolean variable that contains the value `.TRUE.` upon successful read in

The type of the returned of value, `x`, is depending on the function. The following functions are declared in the `DefUtils` module:

- A value of type `REAL` is read in using the function

```
REAL(KIND=dp) :: r
...
r = GetConstReal( List, Name, Found )
```

- A variable of type `INTEGER` is read in using the function

  ```
  INTEGER :: i
  ...
  i = GetInteger( List, Name, Found )
  ```

- A string is read into a user function or solver by the following code line

  ```
  CHARACTER(LEN=MAX_NAME_LEN) :: str
  ...
  str = GetString( List, Name, Found )
  ```

It is important to note that these routines are only meant for reading in constant values. Consequently, these values must not be dependent on other variables.

Reading Mesh-values from the Solver Input File

The previously introduced function `GetConstReal` is defined for reading in a constant value of type `REAL(KIND=dp)`. In the case if values have to be obtained for nodes of an element defined on the mesh (e.g., an initial condition, a boundary condition or a material parameter), the following function has to be used

```
FUNCTION GetReal( List, Name, Found, UElement ) RESULT(x)
   TYPE(ValueList_t), POINTER :: List
   CHARACTER(LEN=*) :: Name
   LOGICAL, OPTIONAL :: Found
   TYPE(Element_t), OPTIONAL, TARGET :: UElement
   REAL(KIND=dp) :: x(CurrentModel % CurrentElement % Type % NumberOfNodes)
```

The returned value, `x`, is a one-dimensional array of type `REAL(KIND=dp)` with entries for every node of the either given element `UElement` or alternatively the default structure `CurrentModel % CurrentElement`. For instance, reading in the material parameter `Viscosity` from an already assigned pointer of type `ValueList_t` for a given element, `Element`, is done by the following code lines

```
REAL(KIND=dp), ALLOCATABLE :: viscosity(:)
INTEGER :: NoNodes
TYPE(ValueList_t), POINTER :: Material
TYPE(Element_t), POINTER :: Element
LOGICAL :: Found
...
allocate viscosity, set pointers Material and Element
...
NoNodes = GetElementNOFNodes(Element)
...
viscosity(1:NoNodes) = GetReal(Material, 'Viscosity', Found, Element)
```

The user has to make sure that the array that later contains the nodal values is of sufficient size. This, for instance, can be guaranteed by allocating it to the maximal occurring number of nodes for an element in the model

```
ALLOCATE(viscosity(CurrentModel % MaxElementNodes))
```

Physical Time as Argument of User Function

If a user function needs physical time as an input, it can be passed as an argument. For instance, if a boundary condition for the normal component of the velocity would have the physical time as the input variable, the function call in the solver input file then would look as follows (see section 11.3 for more details on user functions)

```
Boundary Condition BCNo
  Name = "time_dependent_outlet"
  Target Boundaries = BoundaryNo
  Normal-Tangential Velocity = True
  Velocity 2 = 0.0
  Velocity 1
   Variable Time
   Real Procedure  "executable" "timeOutletCondition"
  End
End
```

Here the entries *BCNo* and *BoundaryNo* have to be replaced by the correct boundary condition and boundary target number. The file *executable* should contain the compiled user function `timeOutletCondition`.

11.2.2 How to Communicate with Structures Inside Elmer Solver

Often it is necessary to get information from inside the Elmer Solver, such as mesh coordinates or field variables associated to another solver procedure. If writing a solver subroutine, all information of that kind is accessible via the type `TYPE(Solver_t) :: Solver`. In the case of a user function (boundary condition, initial condition, material parameter), the default structure `CurrentModel % Solver` has to be used.

Inquiring Information on the Element

As mentioned earlier, most of the pre-defined functions and subroutines inside Elmer Solver apply on the whole element rather than on single nodes. Information on elements can be accessed via the pre-defined type `Element_t`. We list the functions/subroutines for the mostly needed purposes:

- Setting the active element (bulk):

  ```
  TYPE(Element_t), POINTER :: Element
  Type(Solver_t), Target :: Solver
  INTEGER :: ElementNumber
  ...
  Element => GetActiveElement(ElementNumber)
  ```

  The argument `Solver` is optional. If it is not given, `CurrentModel % Solver` is used. This function also automatically sets the pointer `CurrentModel % CurrentElement` to the element with the given element number `ElementNumber`. This is important if sub-sequentially called functions rely on this default value to be set.

  The total number of active bulk elements for a specific solver is to be inquired using the value `Solver % NumberOfActiveElements`.

- Setting the active element (boundary):

  ```
  TYPE(Element_t), POINTER :: BoundaryElement
  INTEGER :: ElementNumber
  ...
  BoundaryElement => GetBoundaryElement(ElementNumber)
  ```

This routine also sets the structure `CurrentModel % CurrentElement` to the boundary element.

In contrary to the domain (i.e., bulk) it is a priory not known which boundary element is part of a boundary condition of a specific solver. This information may be obtained using the function

```
Type(Element_) :: BoundaryElement
LOGICAL :: IsActiveBoundary
...
IsActiveBoundary = BoundaryElement(BoundaryElement,Solver)
```

where both arguments are optional. If they are omitted, Elmer Solver takes the values `CurrentModel % CurrentElement` and `CurrentModel % Solver`, respectively. The boundary element number, `ElementNumber` may vary between 1 and the maximum value

```
Solver % Mesh % NumberOfBoundaryElements
```

- Inquire number of nodes in an element:

```
INTEGER :: N
TYPE(Element_t) :: Element
...
N = GetElementNOFNodes( Element )
```

The argument `Element` is optional. The default value is `CurrentModel % CurrentElement`

- Get nodal coordinates for element:

```
TYPE(Nodes_t) :: ElementNodes
TYPE(Element_t) :: Element
TYPE(Solver_t) :: Solver
...
CALL GetElementNodes( ElementNodes, Element, Solver )
```

The arguments `Element` and `Solver` are optional. The default values are `CurrentModel % CurrentElement` and `CurrentModel % Solver`, respectively. The argument `ElementNodes` is of the pre-defined type `Nodes_t`. The different components of the coordinates for the i-th node can be accessed by

```
REAL(KIND=dp) :: Xcoord, Ycoord, Zcoord
...
Xcoord = ElementNodes % x(i)
Ycoord = ElementNodes % y(i)
Zcoord = ElementNodes % z(i)
```

They correspond to the axes of the defined coordinate system in the solver input file.

- Get local coordinates of the `i`-th node for assigned element:

```
REAL(KIND=dp) :: U, V, W
TYPE(Element_t), POINTER :: Element
INTEGER :: i
...
U = Element % Type % NodeU(i)
V = Element % Type % NodeV(i)
W = Element % Type % NodeW(i)
```

Local coordinates are corresponding to the position inside the prototype element that is used inside the Elmer Solver. They are important if parameter values have to be obtained by summation over the basis functions.

- Get normal vector at the `i`-th node of the assigned boundary element:

  ```
  REAL(KIND=dp) :: U, V, Normal(3)
  TYPE(Element_t), POINTER :: BoundaryElement
  LOGICAL :: CheckDirection
  ...
  U = BoundaryElement % Type % NodeU(i)
  V = BoundaryElement % Type % NodeV(i)
  Normal = NormalVector( BoundaryElement, Nodes, U, V, CheckDirection )
  ```

  The function needs the boundary element as well as the local coordinates of the point, where the surface (edge) normal shall be evaluated. The optional last argument, `CheckDirection`, is a boolean variable. If set to `.TRUE.`, the direction of the normal is set correctly to the rules given in section 11.3.2. The surface normal is returned in model coordinates and is of unity length.

Inquiring Nodal Values of Field Variables

Nodal values for an element of a scalar variables are read by the subroutine

```
SUBROUTINE GetScalarLocalSolution( x,name,UElement,USolver )
     REAL(KIND=dp) :: x(:)
     CHARACTER(LEN=*), OPTIONAL :: name
     TYPE(Solver_t)  , OPTIONAL, TARGET :: USolver
     TYPE(Element_t),  OPTIONAL, TARGET :: UElement
```

The returned value is an array containing the nodal values of the variable `name`. If this variable name is not provided, it is assumed that the corresponding solver `USolver` has only one variable with a single degree of freedom. If the optional parameters `USolver` and `UElement` are not provided, then the default values `CurrentModel % Solver` and `CurrentModel % CurrentElement`, respectively, are used.

For instance, the following code lines read in the nodal element values for the variable `Temperature` (from the heat solver)

```
REAL(KIND=dp), ALLOCATABLE :: localTemp(:)
ALLOCATE(localTemp(CurrentModel % MaxElementNodes))
...
CALL GetScalarLocalSolution(localTemp, 'Temperature')
```

In the case of a vector field variable, the analog function `GetVectorLocalSolution` has to be used. For instance, if the user wants to read in the local velocity of an deforming mesh (from the MeshSolver), the following syntax has to be applied

```
REAL(KIND=dp) , ALLOCATABLE :: localMeshVelocity(:,:)
ALLOCATE(localMeshVelocity(3,Solver % Mesh % MaxElementNodes)
...
CALL GetVectorLocalSolution( MeshVelocity, 'Mesh Velocity')
```

Inquiring Values of Field Variables for the Whole Mesh

Sometimes, the user also would like to have values for a field variable of the complete domain accessible. This is done by assigning a pointer to the variable using the function `VariableGet`

```
VariablePointer => VariableGet(Solver % Mesh % Variables, 'Variable' )
```

The argument *`Variable`* has to be replaced by the variable name. The returned pointer is of type `Variable_t`. This type contains the following components

component	purpose
`INTEGER, POINTER :: Perm(:)`	Contains permutations for the variable. Since Elmer Solver tries to optimize the matrix structure, the numbering of the nodal values of the variable usually does not coincide with the numbering of the mesh-nodes. The is used to identify the mesh-node for a variable-entry. Hence, the field `VariablePointer % Perm(i)` contains the nodal number of the `i`-th value of the field variable *`Variable`*.
`INTEGER :: DOFs`	Contains the amount of vector components of the variable. `DOFs` is 1 in case of a scalar, 2 or 3 in case of a two- or three-dimensional vector field.
`REAL(KIND=dp), POINTER :: Values(:)`	contains the values of the field variable

For instance, in order to get access to the temperature field (similar as in the example above), the following code lines may be used

```
TYPE(Variable_t), POINTER :: TempVar
INTEGER, POINTER :: TempPerm(:)
REAL(KIND=dp), POINTER :: Temperature(:)
INTEGER :: ElmentNo, N
REAL(KIND=dp), ALLOCATABLE :: localTemp(:)
ALLOCATE(localTemp(CurrentModel % MaxElementNodes))
TYPE(Element_t), POINTER :: Element
...
TempVar => VariableGet( Solver % Mesh % Variables, 'Temperature' )
IF ( ASSOCIATED( TempVar) ) THEN
  TempPerm    => TempVar % Perm
  Temperature => TempVar % Values
!!!! stop if temperature field has not been found !!!!
ELSE IF
  CALL Fatal('MyOwnSolver', 'No variable Temperature found')
END IF
...
DO ElementNo = 1,Solver % NumberOfActiveElements
   Element => GetActiveElement(ElementNo)
   N = GetElementNOFNodes()
   NodeIndexes => Element % NodeIndexes
   localTemp(1:N) = Temperature(TempPerm(Element % NodeIndexes))
END DO
```

It is recommended to check whether the pointer to the variable has been assigned correctly. In our little example the call of the routine `Fatal` would stop the simulation run if the assessment would lead to a negative result.

Inquiring the Current Time

In certain situations in transient simulations the physical time might be needed in a user function. In Elmer Solver the physical time is treated as a variable and hence has to be read in using the type `Variable_t`

```
TYPE(Variable_t), POINTER :: TimeVar
Real(KIND=dp) :: Time
...
TimeVar => VariableGet( Solver % Mesh % Variables, 'Time' )
Time = TimeVar % Values(1)
```

How to Post Messages

Including `PRINT` or `WRITE` statements to stdio in numeric-codes can lead excessive output (large number of iterations and/or large model sizes) and consequently to a reduction in performance. It is recommended to use stdio-output routines provided by Elmer Solver, for which to a certain extend the amount of output can be controlled via the solver input file. The three pre-defined subroutines for output of messages are:

- `Info` is used for displaying messages (e.g., upon convergence) on the screen. The syntax is

  ```
  CALL Info('FunctionName','The displayed message', level=levelnumber)
  ```

  The first string shall indicate which function the displayed message comes from. The second entry is a string that contains the message itself. The integer value *`levelnumber`* indicates the importance of the message, starting from 1 (most important). The maximum level of messages being displayed can be determined in the simulation section of the solver input file

  ```
  max output level = 3
  ```

- `Warn` is used for displaying warnings. Warnings are always displayed and should be used if conditions in the code occur that might lead to possible errors

  ```
  CALL Warn('FunctionName','The displayed warning')
  ```

- `Fatal` is used to terminate the simulation displaying a message. Consequently, it is used in conditions in the code where a continuation of the computation is impossible

  ```
  CALL Fatal('FunctionName','The displayed error message')
  ```

Of course the strings do not have to be hard-coded but can be composed during run-time, using the `WRITE` command. The string variable `Message` is provided for that purpose

```
WRITE(Message,formatstring) list, of, variables
CALL Info('FunctionName',Message, level=3)
```

The format-string has to be set according to the list of variables.

11.3 Writing a User Function

User functions can be used to provide a pointwise (not element wise!) value for a certain property. They are used for setting values of material properties inside the domain and/or to set values for certain variables on boundary conditions at the domain boundary.

The defined interface for a user function looks as follows

```
FUNCTION myfunction( model, n, var ) RESULT(result)
  USE DefUtils
  IMPLICIT None
  TYPE(Model_t) :: model
  INTEGER :: n
  REAL(KIND=dp) :: var, result

  ... contents of the function
  leading to a value for variable result ...

END FUNCTION myfunction
```

The function returns the value `result`. If this is supposed to be a nodal value of a material property or a variable condition, the variable type in Elmer has to be real double precision, hence, `REAL(KIND=dp)`.
The first argument passed to the function, `model`, is of the declared type `Model_t`. It is basically the interface to all information accessible at runtime, such as variable values, mesh coordinates and boundary conditions.
The second argument, `n`, is the integer number of the node for which the function - i.e., the value `result` - is is evaluated. Through the last argument, `var`, a value of an input variable on which the result depends is passed to the function. In the solver input file this variable is indicated using the `Variable`-keyword. For instance (see examples later in this chapter), if the user wants to provide the function above with the result being the density which – in this particular case – depends on the temperature, the syntax looks as follows

```
Density  = Variable Temperature
  Procedure "filename" "myfunction"
```

Mind that there always has to be an input variable to be given using this keyword. In the case that there is no need for an input, this may occur as a dummy argument in the function.

11.3.1 User Functions for Domain Properties

In the following we will give an outline of the main issues concerning the preparation of a user function for a domain property. This might be of use if a material parameter (from material section of the solver input file), an initial condition (from solver input file initial condition section) or a body force (from solver input file body force section) of somewhat higher complexity has to be defined for the domain.

Some basic aspects concerning the syntax of such functions shall be explained by the following examples:

Example: Viscosity as a Function of Temperature

This example demonstrates the following topics:

- definition of a material property dependent on one input variable
- how to read in a value from the material section of the solver input file

We want to implement the following relation for the dynamic viscosity, μ, of a fluid

$$\mu(T) = \mu_{293\mathrm{K}}\ \exp\left[C \cdot \left(\frac{293}{T} - 1\right)\right] \tag{11.1}$$

where T is the temperature. The parameters $\mu_{293\mathrm{K}}$ (i.e., the reference viscosity at 293 Kelvin) and C have to be read into our function from the material section of the solver input file. Thus, the material section looks as follows:

```
! Material section (ethanol)
! --------------------------
Material 1
  ...
  Viscosity = Variable Temperature
  Procedure "fluidproperties" "getViscosity"
  ...
  Reference Viscosity = Real 1.2E-03
  Parameter C = Real 5.72
  ...
End
```

The values $\mu_{293\mathrm{K}} = 1.2 \cdot 10^{-3}$ and $C = 5.72$ are the numerical values of the parameter occurring in (11.1) for pure ethanol. The executable containing the function named `getViscosity` will be called `fluidproperties`. The header – including the variable declaration – of the function then reads as follows:

```
!-----------------------------------------------------
! material property function for ELMER:
! dynamic fluid viscosity as a function of temperature
!-----------------------------------------------------
FUNCTION getViscosity( model, n, temp ) RESULT(visc)
  ! modules needed
  USE DefUtils

  IMPLICIT None

  ! variables in function header
  TYPE(Model_t) :: model
  INTEGER :: n
  REAL(KIND=dp) :: temp, visc

  ! variables needed inside function
  REAL(KIND=dp) :: refVisc, C
  Logical :: GotIt
  TYPE(ValueList_t), POINTER :: material
```

In order to get the pointer to the correct material-list, we use the function `GetMaterial`

```
  ! get pointer on list for material
  material => GetMaterial()
  IF (.NOT. ASSOCIATED(material)) THEN
     CALL Fatal('getViscosity', 'No material found')
  END IF
```

We immediately check, whether the pointer assignment was successful. In the case of the NULL-pointer being returned, the pre-defined procedure `Fatal` will stop the simulation and stdio will display the the message: `(getViscosity):  No material-id found`
The next step is to read in the numerical values for the parameter:

```
  ! read in reference viscosity
  refvisc = GetConstReal( material, 'Reference Viscosity', GotIt)
  IF(.NOT. GotIt) THEN
     CALL Fatal('getViscosity', 'Reference Viscosity not found')
  END IF

  ! read in parameter C
  C = GetConstReal( material, 'Parameter C', GotIt)
  IF(.NOT. GotIt) THEN
     CALL Fatal('getViscosity', 'Parameter C not found')
  END IF
```

The variable `GotIt` contains the state of success of the input. In the case of unsuccessful read-in (i.e., the variable `GotIt` shows the value `.FALSE.`), the simulation will be stopped by the routine `Fatal`.
Finally, after a check upon the absolute temperature being larger than zero, the viscosity is computed according to equation (11.1)

```
  ! compute viscosity
  IF (temp <= 0.0D00) THEN ! check for physical reasonable temperature
     CALL Warn('getViscosity', 'Negative absolute temperature.')
     CALL Warn('getViscosity', 'Using viscosity reference value')
     visc = refVisc(1)
  ELSE
```

```
     visc = refVisc * EXP(C *(2.93D02/temp - 1.0D00))
  END IF

END FUNCTION getViscosity
```

In the case of negative absolute temperature, the reference value will be returned. The pre-defined routine `Warn` will display a specific warning on stdio.

Example: Body Force as a Function of Space

For the use as body force for the solver presented in 11.4 (i.e. heat source distribution for heat conduction equation), we want to write a function that provides a scalar in the domain as a function of space. This example demonstrates the following topics:

- definition of a scalar in the domain as function of space in two dimensions
- how to inquire the dimension of the problem

We want to implement the following two-dimensional spatial distribution for the scalar h:

$$h(x,y) = -\cos(2\,\pi\,x)\cdot\sin(2\,\pi\,y), \quad x,y \in [0,1] \tag{11.2}$$

where x corresponds to `Coordinate 1` and y to `Coordinate 2` of the solver input file.

Since the function given in (11.2) is dependent on two input variables, the single argument that is able to be passed to the function is not sufficient. Hence it will just be used as dummy argument. Consequently, the user can provide any (existing!) variable as argument in the solver input file. The header reads as follows

```
!------------------------------------------------------
! body force function for ELMER:
!   scalar load as function of coordinates x and y
!               -cos(2*pi*x)*sin(2*pi*y)
!------------------------------------------------------
FUNCTION getLoad( model, n, dummyArgument ) RESULT(load)
  ! modules needed
  USE DefUtils

  IMPLICIT None

  ! variables in function header
  TYPE(Model_t) :: model
  INTEGER :: n
  REAL(KIND=dp) :: dummyArgument, load

  ! variables needed inside function
  INTEGER :: DIM
  REAL(KIND=dp) :: x, y
  Logical :: FirstVisited = .TRUE.

  ! remember these variables
  SAVE DIM, FirstVisited
```

Further we want to check whether the problem is two-dimensional and hence suitable for our function. This is done only the first time the function is called, since - hopefully - the dimension of the problem does not change during all the following calls. The function returning the problem dimension is `CoordinateSystemDimension()`

```
  ! things done only the first time the function is visited
  IF (FirstVisited) THEN
```

```
     ! check whether we are dealing with a 2d model
     DIM = CoordinateSystemDimension()
     IF (DIM /= 2) THEN
        CALL FATAL('getLoad', 'Dimension of model has to be 2d')
     END IF
     FirstVisited = .FALSE.
  END IF
```

The next step to inquire the coordinates of the current point the function is evaluated for. The structure `model` contains that information

```
  ! get the local coordinates of the point
  x = model % Nodes % x(n)
  y = model % Nodes % y(n)
```

Finally, the result is computed

```
  ! compute load
  load = -COS(2.0D00*PI*x) * SIN(2.0D00*PI*y)

END FUNCTION getLoad
```

Figure 11.2 shows the result of a simulation using the solver defined in section 11.4 together with the function `getLoad` as body force. The entry in the body force section of the solver input file reads as follows:

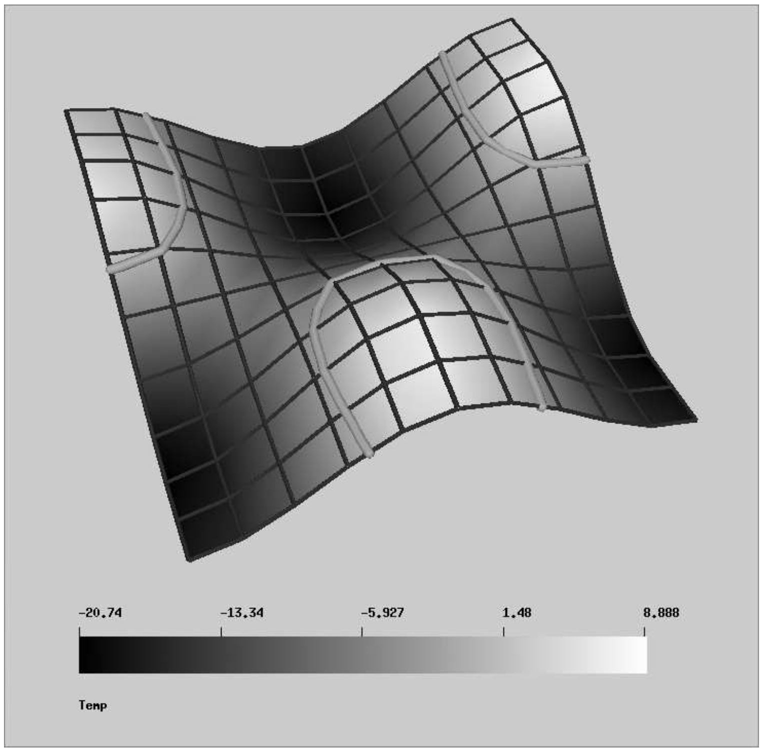


Figure 11.2: Result obtained with the routine `getLoad` as body force input for the heat conduction solver presented in 11.4. The z-coordinate is set proportional to the result obtained in the x-y plane.

```
Body Force 1
  Heat Source
   Variable Temp      !just a dummy argument
   Real Procedure "load" "getLoad"
End
```

where the shared object file has been given the name `load`. All boundaries are set to adiabatic boundary condition, i.e., $\nabla T \cdot \vec{n} = 0$. This is possible if – and only if – the integral over the load vector over the whole domain balances to zero, like in our case. Since no Dirichtlet condition is set, the result is not unique and contains an undetermined offset T_0.

11.3.2 User Functions for Boundary Conditions

As for the user functions for bulk properties presented in section 11.3.1, the function for a boundary property is evaluated pointwise. Hence, the identical function interface is used. The major difference between bulk elements and elements on boundaries are, that the latter can be associated to more than one body. That is the case on boundaries between bodies. This is important in such cases where the boundary condition is dependent on properties inside a specific body to which the boundary is attached. Possible configurations of boundaries are depicted in Fig. 11.3.

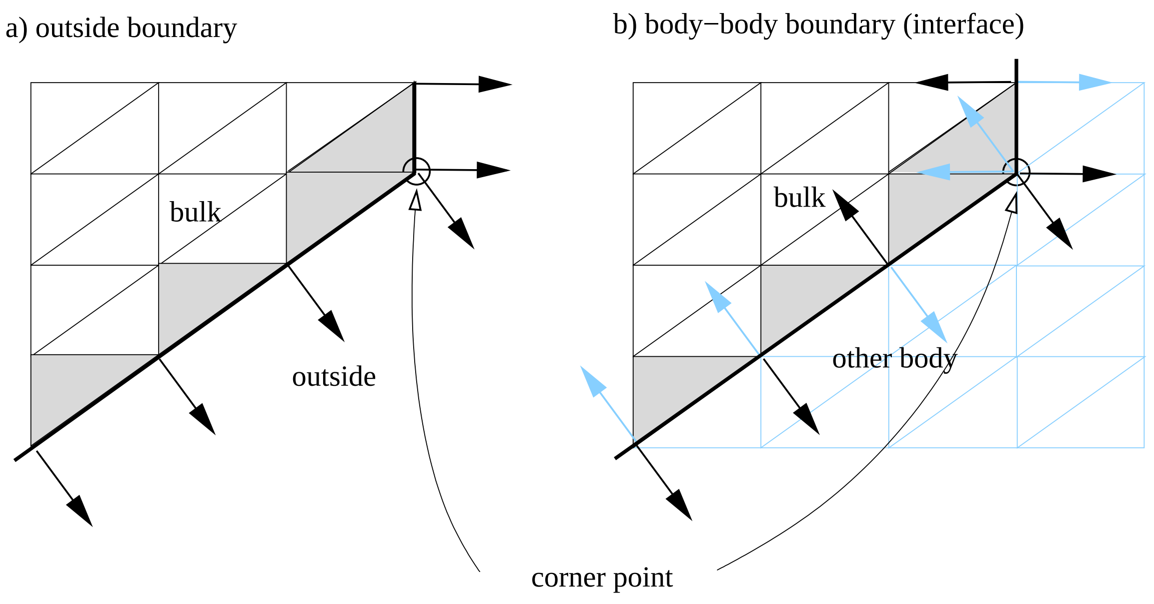


Figure 11.3: Possible constellations for boundaries and the normal vectors, $\vec{n}$ at element nodes. Mind, that for a body-body interface (case b) the default orientation of the surface normal may vary from element to element. At boundary points that have a discontinuous first derivative of the surface (i.e. at corners and edges), the evaluation of the normal at the same point for two adjacent boundary elements leads to different surface normals. Parent elements of boundary elements for the specific body are marked as filled.

If the keyword for checking the directions in the function `NormalVector` (see section 11.2.2) is set to `.TRUE.`, the following rules apply:

- In the case of an outside boundary the surface normal, $\vec{n}$, is always pointing outwards of the body.
- By default on a body-body boundary, the orientation is such that the normal always is pointing towards the body with lower density, ϱ, which is evaluated by comparison of the values given for the keyword `Density` in the corresponding material sections of the adjacent bodies.

In certain cases, if densities on both sides are either equal or varying functions of other variables, this may lead to a varying orientation of the surface. This effect and the effect of different directions of surface normal for the same point at surface corners and edges is depicted in Fig. 11.3. Whereas the latter effect can only be dealt with by either producing smooth surfaces or averaging surface normals, the first problem can be overcome by providing the keyword `Normal Target Body` in the solver input file. This keyword defines the direction of the surface normals for the pre-defined subroutine `NormalVector`. For instance, the following sequence fixes the surface normal at boundary condition number 1 to point into body number 2

```
Boundary Condition 1
  Target Boundaries = 1
  Normal Target Body = Integer 2
...
End
```

Example: Idealized Radiation Law for External Heat Transfer

As an illustrative example we want to show how to implement a very idealized radiation boundary condition for heat transfer. This example explains:

- how to identify the type of boundary according to Fig. 11.3
- how to get material parameters from domain parent elements of the boundary element
- how to identify the local node number in an elment
- how to inquire boundary normals

The net flux into the body at such a boundary shall be approximated by

$$q_n = \epsilon\, q_{\mathrm{ext}} - \epsilon\sigma \cdot \left(T^4 - T_{\mathrm{ext}}^4\right), \tag{11.3a}$$

where T_{ext} is the external temperature, σ stands for the Stefan-Boltzmann constant and ϵ is the emissivity. The external heat flux shall be defined as

$$q_{\mathrm{ext}} = \begin{cases} -I\vec{s}\cdot\vec{n}, & \vec{s}\cdot\vec{n} < 0, \\ 0, & \text{else}, \end{cases} \tag{11.3b}$$

where I is the intensity and $\vec{s}$ the direction of the incoming radiation vector. The surface normal, $\vec{n}$, is assumed to point outwards the body surface.

Since we are planning to use this boundary condition in connection with the solver presented in section 11.4.2, we have to provide the load vector $l = q_n/(c_p\,\varrho)$ occurring in the force vector of (11.7). This means that we have to inquire the material parameters c_p and ϱ for the parent element from the material section of the adjacent body.

The header of the function reads as

```
!------------------------------------------------------
! boundary condition function for ELMER:
!  simplified radiation BC
!------------------------------------------------------
FUNCTION simpleRadiation( model, n, temp ) RESULT(load)
  ! modules needed
  USE DefUtils

  IMPLICIT None

  ! variables in function header
  TYPE(Model_t) :: model
  INTEGER :: n
  REAL(KIND=dp) :: temp, load

  ! variables needed inside function
  REAL(KIND=dp), ALLOCATABLE :: Density(:), HeatCapacity(:), ExtTemp(:)
  REAL(KIND=dp), POINTER :: Work(:,:)
  REAL(KIND=dp) :: radvec(3), Normal(3), NormDir, U, V,&
       Emissivity, normalabsorbtion, emission, StefanBoltzmann
  INTEGER :: DIM, other_body_id, nboundary, nparent,&
       BoundaryElementNode, ParentElementNode, istat
  Logical :: GotIt, FirstTime=.TRUE., Absorption = .TRUE.
  TYPE(ValueList_t), POINTER :: ParentMaterial, BC
  TYPE(Element_t), POINTER :: BoundaryElement, ParentElement
  TYPE(Nodes_t) :: ElementNodes

  SAVE FirstTime, Density, HeatCapacity, ExtTemp
!------------------------------------------------------------------------
```

The boundary element and the pointer to the list of the corresponding Boundary Condition-entry in the solver input file are assigned

```
! ----------------------
! get element information
! ----------------------
  BoundaryElement => CurrentModel % CurrentElement
  IF ( .NOT. ASSOCIATED(BoundaryElement) ) THEN
     CALL FATAL('simpleRadiation','No boundary element found')
  END IF

  BC => GetBC()
  IF ( .NOT. ASSOCIATED(BC) ) THEN
     CALL FATAL('simpleRadiation','No boundary condition found')
  END IF
```

Thereafter, a case distinction between the two possible constellations in Fig. 11.3 (i.e.,outside or body-body boundary). A outside boundary is indicated by the value -1 of `BoundaryElement % BoundaryInfo % outbody`. In the case of a boundary-boundary interface the surface normal is supposed to point outwards. I.e., the body hosting the parent element is taken the one for which `ParentElement % BodyId` does not coincide with `BoundaryElement % BoundaryInfo % outbody`

```
  other_body_id = BoundaryElement % BoundaryInfo % outbody
  ! only one body in simulation
  ! -------------------------
  IF (other_body_id < 1) THEN
     ParentElement => BoundaryElement % BoundaryInfo % Right
     IF ( .NOT. ASSOCIATED(ParentElement) )&
          ParentElement => BoundaryElement % BoundaryInfo % Left
  ! we are dealing with a body-body boundary
  ! and assume that the normal is pointing outwards
  ! ---------------------------------------------
  ELSE
     ParentElement => BoundaryElement % BoundaryInfo % Right
     IF (ParentElement % BodyId == other_body_id)&
          ParentElement => BoundaryElement % BoundaryInfo % Left
  END IF

  ! just to be on the save side, check again
  ! --------------------------------------
  IF ( .NOT. ASSOCIATED(ParentElement) ) THEN
     WRITE(Message, *)&
```

```
          'No parent element found for boundary element no. ', n
     CALL FATAL('simpleRadiation',Message)
  END IF
```

After that procedure the pointer `ParentElement` is set on the adjacent element of the boundary element inside the body for which the radiation boundary condition is evaluated.

We further need the total number of nodes in the boundary element and the parent element given by `nboundary` and `nparent`, respectively. Also the corresponding number of the boundary node number, `n`, in the parent element, `ParentElementNode`, as well as in the boundary element itself, `BoundaryElementNode`, is evaluated. At the end of this code sequence, the routine `GetElementNodes` sets the information on the nodes of the boundary element

```
  ! get the corresponding node in the elements
  ! -----------------------------------------
  nboundary = GetElementNOFNodes(BoundaryElement)
  DO BoundaryElementNode=1,nboundary
     IF (  n == BoundaryElement % NodeIndexes(BoundaryElementNode) ) EXIT
  END DO
  nparent = GetElementNOFNodes(ParentElement)
  DO ParentElementNode=1,nboundary
     IF (  n == ParentElement % NodeIndexes(ParentElementNode) ) EXIT
  END DO

  ! get element nodes
  ! -----------------
  CALL GetElementNodes(ElementNodes, BoundaryElement)
```

The needed space for reading material parameter fro the parent element as well as boundary condition parameters for the boundary element is allocated. In the case of the function being re-visited, we first do a deallocation, since the values of `nboundary` or `nparent` may change from element to element (hybrid mesh)

```
! -----------
! Allocations
! -----------
  IF (.NOT.FirstTime) THEN
     DEALLOCATE(Density, HeatCapacity, ExtTemp)
  ELSE
     FirstTime = .FALSE.
  END IF
  ALLOCATE(Density( nparent ), HeatCapacity( nparent ),&
       ExtTemp(nboundary), stat=istat)
  IF (istat /= 0) CALL FATAL('simpleRadiation', 'Allocations failed')
```

The following code lines read the values for the parameters associated with the boundary element and the Stefan-Boltzmann constant from the solver input file

```
! ----------------------------------------
! get parameters from constants section
!     and boundary condition section
! ----------------------------------------
  DIM = CoordinateSystemDimension()
  StefanBoltzmann = ListGetConstReal( Model % Constants, &
       'Stefan Boltzmann',GotIt)
  IF (.NOT. GotIt) THEN ! default value in SI units
     StefanBoltzmann = 5.6704D-08
  END IF
  Emissivity = GetConstReal( BC,'Emissivity',GotIt)
  IF ((.NOT. GotIt) .OR. &
   ((Emissivity < 0.0d0) .OR. (Emissivity > 1.0d0))) THEN
     load = 0.0d00
     CALL WARN('simpleRadiation','No Emissivity found.')
     RETURN ! no flux without or with unphysical emissivity
  END IF

  ExtTemp(1:nboundary) = GetReal( BC,'External Temperature',GotIt)
  IF (.NOT.GotIt) THEN
     WRITE (Message,*) 'No external temperature defined at point no. ', n
     CALL Warn('simpleRadiation', Message)
     ExtTemp(1::nboundary)= temp
  END IF

  Work => ListGetConstRealArray( BC,'Radiation Vector',GotIt)
  IF ( GotIt ) THEN
     radvec = 0.0D00
     NormDir =  SQRT(SUM(Work(1:DIM,1) * Work(1:DIM,1)))
     IF (NormDir /= 0.0d00) THEN
        radvec(1:DIM) = Work(1:DIM,1)*Work(4,1)/NormDir
     ELSE ! no radiation for weird radiation vector
        Absorption = .FALSE.
     END IF
  ELSE ! no absorption without radiation vector
     Absorption = .FALSE.
  END IF
```

If absorption of an incoming radiation vector has to be computed, the surface normal has to be inquired

```
! --------------------------------
! get surface normals ( if needed )
! --------------------------------
  IF (Absorption) THEN
     U = BoundaryElement % Type % NodeU(BoundaryElementNode)
     V = BoundaryElement % Type % NodeV(BoundaryElementNode)
     Normal = NormalVector(BoundaryElement, ElementNodes, U, V, .TRUE.)
  END IF
```

Thereafter, the needed material parameters are read from the material section of the solver input file that associated with the body for which the radiation boundary condition is computed

```
! -----------------------------------------
! get material parameters from parent element
! -----------------------------------------
  ParentMaterial => GetMaterial(ParentElement)
  ! next line is needed, if the consequently read
  ! parameters are themselves user functions
  ! ------------------------------------------
  CurrentModel % CurrentElement => ParentElement
  Density(1:nparent) = GetReal(ParentMaterial, 'Density', GotIt)
  IF (.NOT.GotIt) Density(1:nparent) = 1.0d00
  HeatCapacity(1:nparent) = GetReal(ParentMaterial, 'Heat Capacity', GotIt)
  IF (.NOT.GotIt) HeatCapacity(1:nparent) = 1.0d00

  ! put default pointer back to where it belongs
  ! ---------------------------------------------
  CurrentModel % CurrentElement => BoundaryElement
```

Since these material parameters themselves may be given in form of user functions, the default pointer `CurrentModel % CurrentElement` has to be set to the parent element upon call of the function `GetReal`.

Finally the two parts of the total normal heat flux are evaluated. The external load is obtained by dividing this Laue by the inquired values for `Density` and `HeatCapacity`.

```
!------------------------------------
! compute flux and subsequently load
!------------------------------------
  IF (Absorption) THEN
     normalabsorbtion = -1.0D00 & ! since normal pointing outwards
          * Emissivity * DOT_PRODUCT(Normal,radvec)
     IF (normalabsorbtion < 0.0d0) &
          normalabsorbtion = 0.0d00
  ELSE
     normalabsorbtion = 0.0d00
  END IF

  emission = StefanBoltzmann * Emissivity * &
       ( temp**4 - ExtTemp(BoundaryElementNode)**4) &
       / (HeatCapacity(ParentElementNode) * Density(ParentElementNode))

  load = normalabsorbtion + emission

END FUNCTION simpleRadiation
```

Figure 11.4 shows the result of the heat conduction solver presented in section 11.4 in combination with the function `simpleRadiation` as boundary condition on two oppositely directed boundaries (boundary condition no. 1). Since the radiation vector is aligned with the x-direction and hence perpendicular with respect to these two boundaries, the absorption part vanishes for one of these boundaries. For the sake of simplicity, the material parameters ϱ, c_p and k have been set to unity. The corresponding entries of the solver input file for the boundary conditions of the case shown in Fig. 11.4 are:

```
Boundary Condition 1
  Target Boundaries(2) = 1 2
  Boundary Type = String "Heat Flux"
  External Load
        Variable Temp
        Real Procedure "radiation_flux.exe" "simpleRadiation"
  External Temperature = Real -20.0E00
  Radiation Vector(4) = Real -1.0E00 0.0E00  0.0E00  1.0E01
  Emissivity = Real 0.5
End

Boundary Condition 2
  Target Boundaries = 3
  Boundary Type = String "Given Temperature"
  Temp = Real 0
End

Boundary Condition 3
  Target Boundaries = 4
  Boundary Type = String "Adiabatic"
End
```

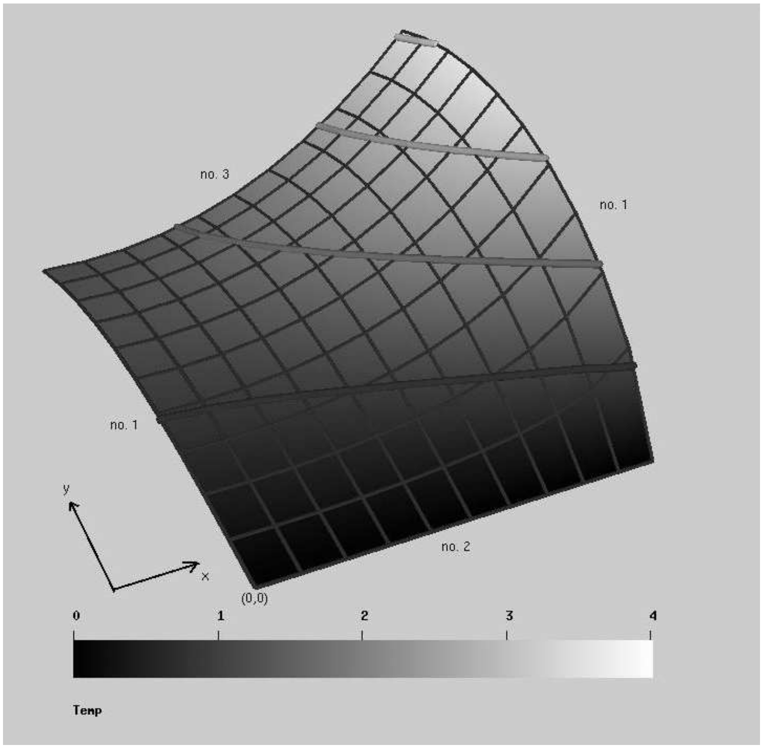


Figure 11.4: Result of the heat conduction solver applying the simplified radiation boundary condition described in this section. The coordinate directions as well as the number of the corresponding boundary condition section are shown. The latter can be compared to the solver input file entries shown in this section.

11.4 Writing a Solver

In Elmer an additional solver may be provided by dynamically linked subroutines. The pre-defined interface of a solver subroutine is

```
SUBROUTINE mysolver( Model,Solver,dt,TransientSimulation )
  TYPE(Model_t) :: Model
  TYPE(Solver_t) :: Solver
  REAL(KIND=dp) :: dt
  LOGICAL :: TransientSimulation
```

The first argument, `Model`, is the same structure also passed to a user function (see section 11.3). The second argument, `Solver`, is of type `Solver_t` and contains all information upon options set for this particular solver. The timestep size, `dt`, and a boolean variable, `TransientSimulation`, indicating whether the solver is to be run as a part of a transient (value `.TRUE.`) or steady state (value .FALSE.) simulation are further arguments of the solver subroutine.

11.4.1 Structure of a Solver

The well known structure of a linearized partial differential equation (PDE) for the scalar T in the variational formulation is

$$\mathbf{M}_{i\,j}\frac{\partial T_j}{\partial t} + \mathbf{A}_{i\,j}T_j = F_i, \tag{11.4}$$

with the mass matrix, $\mathbf{M}_{i\,j}$, the stiffness matrix, $\mathbf{A}_{i\,j}$ and the force vector, F_i.

Time-stepping and the coupled solver iteration – i.e., the steady state or time level iteration of several solvers of the simulation – is taken care of by the main part of the Elmer Solver. The task of the user supplying a user defined solver subroutine is to linearize an eventually nonlinear PDE and to supply the Elmer Solver with the element-wise components for the matrices as well as the force vector.

This leads to a principle structure of a user defined solver subroutine as it is depicted in Fig. 11.5. We further will explain the construction of a user solver subroutine by discussing an example case.

11.4.2 Example: Heat Conduction Equation

In order to provide a simple example, we want to explain how the solution of the purely convective heat transport equation is implemented in Elmer. This example explains:

- reading solver parameters from the solver input file
- assembly of the local element matrix components for the domain and a von Neumann condition including explanation of the most important Elmer Solver routines needed for linear system matrix assembly and solution
- how to deal with non-linear and transient PDE's
- how to implement Dirichlet boundary conditions

For constant density, ϱ, and heat capacity, c_p this equation may be written as

$$\frac{\partial T}{\partial t} - \nabla\cdot\left(\frac{k}{c_p\,\varrho}\,\nabla T\right) = \frac{h}{c_p\,\varrho}, \tag{11.5}$$

where T stands for the temperature, k for the heat conductivity and h is the heat source.

The variational formulation of (11.5) reads after partial integration of the conduction term and application of Green's theorem

$$\int\limits_V \frac{\partial T}{\partial t}\gamma_i\,dV + \int\limits_V \frac{k}{c_p\,\varrho}\,\nabla T\cdot\nabla\gamma_i\,dV = \int\limits_V \frac{h}{c_p\,\varrho}\gamma_i\,dV + \oint\limits_{\partial V}\frac{1}{c_p\,\varrho}\underbrace{(k\,\nabla T)\cdot\vec{n}}_{=q_n}\,\gamma_i\,dA, \tag{11.6}$$

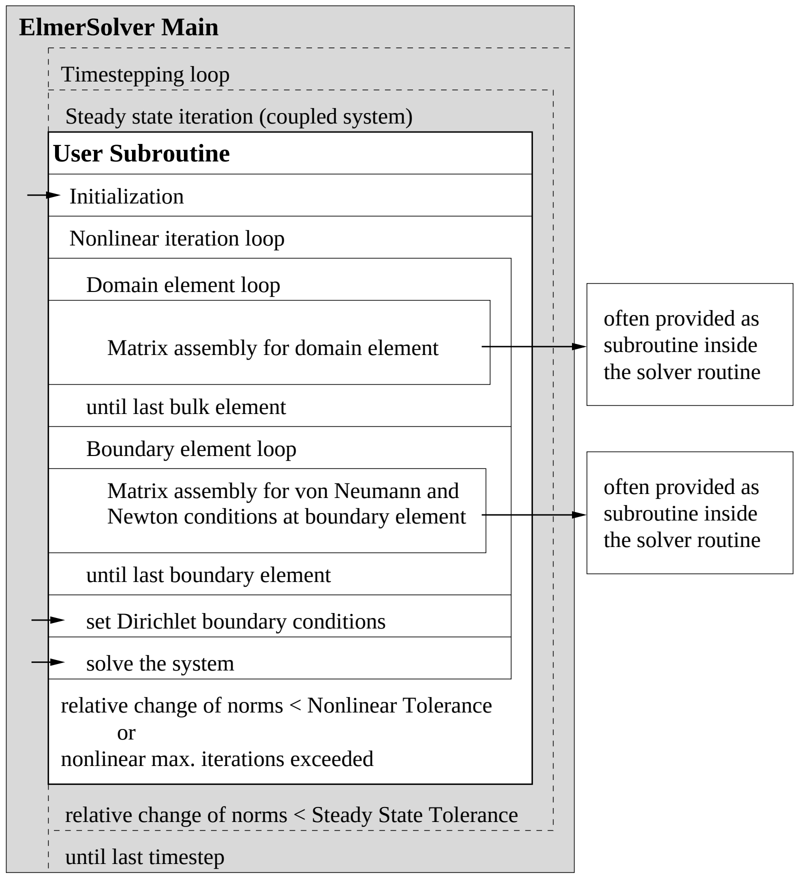

ElmerSolver Main
Timestepping loop
Steady state iteration (coupled system)
User Subroutine
Initialization
Nonlinear iteration loop
Domain element loop
Matrix assembly for domain element
until last bulk element
Boundary element loop
Matrix assembly for von Neumann and Newton conditions at boundary element
until last boundary element
set Dirichlet boundary conditions
solve the system
relative change of norms < Nonlinear Tolerance or nonlinear max. iterations exceeded
relative change of norms < Steady State Tolerance
until last timestep
often provided as subroutine inside the solver routine
often provided as subroutine inside the solver routine

Figure 11.5: Flowchart of a user defined solver subroutine within Elmer Solver. The grey underlayed area indicates the tasks of a simulation that are provided by Elmer, whereas the white area contains the flowchart for the source code of the user subroutine. Arrows pointing into this field indicate needed subroutine/function calls to Elmer Solver.

where γ_i is the basis-function, V and ∂V is the element volume and its enclosing surface, respectively. The surface normal of ∂V is denoted by $\vec{n}$. According to the Galerkin method, the variable is given as $T = T_j\gamma_j$, with the sum taken over the index j. Comparing with (11.4) leads to the matrices and vectors

$$\begin{aligned}
\mathbf{M}_{i\,j} &= \int\limits_V \gamma_j\gamma_i\,dV, \\
\mathbf{A}_{i\,j} &= \int\limits_V \frac{k}{c_p\,\varrho}\nabla\gamma_j\cdot\nabla\gamma_i\,dV, \\
F_i &= \int\limits_V \frac{h}{c_p\,\varrho}\nabla\gamma_i\,dV + \oint\limits_{\partial V}\underbrace{\frac{q_n}{c_p\,\varrho}}_{=l}\gamma_i\,dA.
\end{aligned} \tag{11.7}$$

Although the external heat flux perpendicular to the surface normal, $q_n(T)$, in general is a function of the temperature we want to keep it formal as being prescribed. Hence, only a contribution in the force vector occurs in our formulation. Mind, that a linear or linearized expression of $q_n(T)$ directly could give a contribution to the stiffness matrix at the entries corresponding to boundary nodes. In our approach, even in the case of a linear dependency $q_n(T) \propto T$ we have to iterate the solution because of our treatment of the boundary condition.

The header contains the declaration needed variables – we tried to give them self explaining identifiers. Furthermore, allocations of the needed field arrays are done for the first time the subroutine is visited (checked by the boolean variable `AllocationsDone`). The variable names of these arrays then have to be included in the `SAVE`-statement at the end of the variable declaration block.

```
SUBROUTINE MyHeatSolver( Model,Solver,dt,TransientSimulation )

  USE DefUtils

  IMPLICIT NONE
!-----------------------------------------------------------------
  TYPE(Solver_t) :: Solver
  TYPE(Model_t) :: Model

  REAL(KIND=dp) :: dt
  LOGICAL :: TransientSimulation
!-----------------------------------------------------------------
! Local variables
!-----------------------------------------------------------------
  TYPE(Element_t),POINTER :: Element

  LOGICAL :: AllocationsDone = .FALSE., Found, Converged

  INTEGER :: n, t, istat, other_body_id, iter, NonlinearIter
  REAL(KIND=dp) :: Norm, PrevNorm=0.0d00, NonlinearTol, RelativeChange

  TYPE(ValueList_t), POINTER :: BodyForce, Material, BC, SolverParams
  REAL(KIND=dp), ALLOCATABLE :: MASS(:,:), STIFF(:,:), LOAD(:), FORCE(:)
  REAL(KIND=dp), ALLOCATABLE :: HeatCapacity(:), HeatConductivity(:),&
       Density(:), ExternalTemp(:), TransferCoeff(:), HeatFlux(:)

  CHARACTER(LEN=MAX_NAME_LEN) :: BoundaryType

  SAVE MASS, STIFF, LOAD, FORCE,&
       HeatCapacity, HeatConductivity,&
       Density, ExternalTemp, TransferCoeff, HeatFlux, &
       AllocationsDone, PrevNorm
!-----------------------------------------------------------------

  !Allocate some permanent storage, this is done first time only:
  !---------------------------------------------------------------
  IF ( .NOT. AllocationsDone ) THEN
     N = Solver % Mesh % MaxElementNodes !big enough for elemental arrays
     ALLOCATE( FORCE(N), LOAD(N), MASS(N,N), STIFF(N,N), STAT=istat )
     IF ( istat /= 0 ) THEN
        CALL Fatal( 'MyHeatSolve',&
             'Memory allocation error for matrix/vectors.' )
     END IF
     ALLOCATE( HeatCapacity(N), HeatConductivity(N), Density(N),&
          ExternalTemp(N), TransferCoeff(N), HeatFlux(N), STAT=istat )
     IF ( istat /= 0 ) THEN
        CALL Fatal( 'MyHeatSolve',&
             'Memory allocation error for parameter arrays.' )
     END IF
     AllocationsDone = .TRUE.
  END IF
```

In the next step, information on the nonlinear iteration is being read from the solver section of the solver input file

```
  !Read in solver parameters
  !-------------------------
  SolverParams => GetSolverParams()
  IF (.NOT. ASSOCIATED(SolverParams))&
       CALL FATAL('MyHeatSolve','No Solver section found')
  NonlinearIter = GetInteger(SolverParams, &
                   'Nonlinear System Max Iterations', Found)
  IF ( .NOT.Found ) NonlinearIter = 1
  NonlinearTol  = GetConstReal( SolverParams, &
       'Nonlinear System Convergence Tolerance',    Found )
  IF ( .NOT.Found ) NonlinearTol = 1.0D-03
```

Therafter, the nonlinear iteration loop (outermost loop of the white underlayed area in Fig. 11.5) is started and the linear system solver is initialized (routine `DefaultInitialize`)

```
!-----------------------------------------------------------------
! Nonlinear iteration loop
!-----------------------------------------------------------------
  DO iter=1,NonlinearIter
     Converged = .FALSE.
     WRITE(Message,'(A,I5,A,I5)') 'Nonlinear iteration no.',iter,&
          ' of max. ', NonlinearIter
     CALL INFO('MyHeatSolve',Message,level=1)

     !Initialize the system and do the assembly:
     !------------------------------------------
     CALL DefaultInitialize()
```

The next loop is over all elements in the simulation domain our solver has been assigned to (`Solver % NumberOfActiveElements`). The function `GetActiveElement` inquires the element associated with the element number `t`. This call at the same time also sets the default pointer `CurrentModel % CurrentElement` to that particular element, which is important if subsequently called functions rely on this pointer to be set correctly (see section 11.3). After inquiring the number of nodes the nodal material parameter values $c_p \rightarrow$ `HeatCapacity(1:n)`, $k \rightarrow$ `HeatConductivity(1:n)` and $\varrho \rightarrow$ `Density(1:n)` are read in. If one of these parameters is not found (i.e., `Found == .FALSE.`), a default value of 1 will be set in order to avoid division by zero.

```
!------------------------------------------------------------------
!    Assembly for the domain
!------------------------------------------------------------------
     DO t=1,Solver % NumberOfActiveElements

        ! get element info
        !----------------
        Element => GetActiveElement(t)
        n = GetElementNOFNodes()

        ! get material parameters
        ! ---------------------
        Material => GetMaterial()
        IF (.NOT. ASSOCIATED(Material)) THEN
           WRITE(Message,'(A,I5,A)') &
                'No material for bulk element no. ',t,' found.'
           CALL FATAL('MyHeatSolve',Message)
        END IF
        HeatCapacity(1:n) = GetReal(Material, 'Heat Capacity', Found )
        IF (.NOT. Found) HeatCapacity(1:n) = 1.0D00
        HeatConductivity(1:n) = &
                 GetReal(Material, 'Heat Conductivity', Found )
        IF (.NOT. Found) HeatCapacity(1:n) = 1.0D00
        Density(1:n) = GetReal(Material, 'Density', Found )
        IF (.NOT. Found) Density(1:n) = 1.0D00
```

In order to call the subroutine taking care of the composition of the element matrices and force vector (subroutine `LocalMatrix`), the load vector – in our case the heat source, $h \rightarrow$ `LOAD(1:n)` – has to be read from the body section of the solver input file. In the case of a transient simulation (indicated by `TransientSimulation == .TRUE.`) the first order time discretization is accounted for using the subroutine `Default1stOrderTime`. Mind, that also higher order time discretization routines would be at hand. The local matrix is added to the global coefficient matrix of Elmer Solver calling the subroutine `DefaultUpdateEquations`

```
        !Get load for force vector
        !------------------------
        LOAD = 0.0d0
        BodyForce => GetBodyForce()
        IF ( ASSOCIATED(BodyForce) ) &
             LOAD(1:n) = GetReal( BodyForce, 'Heat Source', Found )

        !Get element local matrix and rhs vector:
        !--------------------------------------
        CALL LocalMatrix( MASS, STIFF, FORCE, LOAD, Element, n,&
             HeatCapacity, HeatConductivity, Density, TransientSimulation)

        !Update global matrix and rhs vector from local matrix & vector:
        !---------------------------------------------------------------
        IF ( TransientSimulation ) THEN
           CALL Default1stOrderTime( MASS,STIFF,FORCE )
        END IF
        CALL DefaultUpdateEquations( STIFF, FORCE )

!-----------------------------------------------------------------
     END DO ! end Assembly for the domain
!-----------------------------------------------------------------
```

After the bulk elements, the contribution to the coefficient matrix and the force vector from a von Neumann type of boundary condition has to be taken into account. To this end, we are looping over all boundary elements. Their total number is given by `Solver % Mesh % NumberOfBoundaryElements`. The routine `ActiveBoundaryElement` checks whether the previously inquired element is part of a boundary condition that has been assigned to our solver. If the value 1 is returned from the function `GetElementFamily` – i.e. we are dealing with boundary element given at a point element – the element also will be skipped, since von Neumann conditions cannot be set on such elements. Finally, the list-pointer to the associated boundary condition section (`GetBC`) is set and the local matrices and vectors are initiated to zero.

```
!-----------------------------------------------------------------
!     assembly of von Neumann boundary conditions
!-----------------------------------------------------------------
     DO t=1, Solver % Mesh % NumberOfBoundaryElements

        ! get element and BC info
        ! ----------------------
        Element => GetBoundaryElement(t)
        IF ( .NOT.ActiveBoundaryElement() ) CYCLE
        n = GetElementNOFNodes()
        ! no evaluation of von Neumann BC’s on points
        IF ( GetElementFamily() == 1 ) CYCLE
        BC => GetBC()

        FORCE = 0.0d00
        MASS = 0.0d00
        STIFF = 0.0d00
```

Since we have to define between different types of boundary conditions, we inquire the contents of a keyword `Boundary Type` from the solver input file. If this string is equal to `’heat flux’`, the variable with the name `’External Load’` will be read in from the boundary condition list `BC`. Thereafter, the contribution to the force vector will be computed by the internal subroutine `BoundaryCondition` (see later in this code). Mind, that the external load is not the given heat flux, q_n, but its value divided by the heat capacity and the density, $l = q_n/(c_p\,\varrho)$. This has to be taken care of if a numerical value or even a user function is provided in the solver input file (see section 11.3.2). In the case of no boundary type being found or an unknown string being detected, the natural boundary condition, zero flux perpendicular to the surface, will be assumed. This is equivalent to the `’adiabatic’` boundary condition. In the case of `’given temperature’` the natural boundary condition will be altered by the matrix manipulation arising from the Dirichlet boundary condition (see later in this code).

```
        ! check type of boundary and set BC accordingly
        !--------------------------------------------------
        BoundaryType = GetString(BC,’Boundary Type’,Found)
        IF (.NOT. Found) CYCLE
        ! natural boundary condition
        IF ((BoundaryType == ’adiabatic’)&
             .OR. (BoundaryType == ’given temperature’)) THEN
           CYCLE
           ! external heat flux
        ELSE IF(BoundaryType == ’heat flux’) THEN
```

```
            ! get external load; mind that this is the heat flux
            ! divided by the density and heat capacity
            LOAD(1:n) = LOAD(1:n) + GetReal(BC,'External Load', Found)
            ! do the assembly of the force vector
            CALL BoundaryCondition(LOAD, FORCE, Element, n)
         ELSE
            WRITE(Message,'(A,I3,A)')&
                 'No boundary condition given for BC no. ',GetBCId(),&
                 '. Setting it to adiabatic.'
            CALL WARN('MyHeatSolve',Message)
            CYCLE
         END IF
```

The boundary element loop is closed after the component system matrix and vector are updated for the current boundary element.

```
         IF ( TransientSimulation ) THEN
            MASS = 0.d0
            CALL Default1stOrderTime( MASS, STIFF, FORCE )
         END IF

         CALL DefaultUpdateEquations( STIFF, FORCE )
!----------------------------------------------------------------
      END DO ! end of assembly of von Neumann boundary conditions
!----------------------------------------------------------------
```

Before setting the Dirichlet conditions (i.e., given boundary temperature T) using the subroutine `DefaultDirichletBCs()` it is important to finish the element-wise assembly of the Elmer Solver system matrix calling `DefaultFinishAssembly`

```
      CALL DefaultFinishAssembly()

      ! call Elmer Solver routine for Dirichlet BCs
      ! ------------------------------------------
      CALL DefaultDirichletBCs()
```

The system is solved by the function call `DefaultSolve`, which returns the norm, N^n of the solution vector T_j for the n-th nonlinear iteration step. This is needed in order to inquire the change of the solution between two steps. If the relative norm

$$R = 2\frac{|N^{n-1} - N^n|}{N^{n-1} + N^n},$$

is smaller than the given tolerance `Nonlinear System Tolerance` of the solver section, then the nonlinear iteration is taken to be converged.

```
      ! Solve the system
      ! ----------------
      Norm = DefaultSolve()

      ! compute relative change of norm
      ! ------------------------------
      IF ( PrevNorm + Norm /= 0.0d0 ) THEN
         RelativeChange = 2.0d0 * ABS( PrevNorm-Norm ) / (PrevNorm + Norm)
      ELSE
         RelativeChange = 0.0d0
      END IF
```

```
     WRITE( Message, * ) 'Result Norm   : ',Norm
     CALL Info( 'MyHeatSolve', Message, Level=4 )
     WRITE( Message, * ) 'Relative Change : ',RelativeChange
     CALL Info( 'MyHeatSolve', Message, Level=4 )


     ! do we have to do another round?
     ! -----------------------------
     IF ( RelativeChange < NonlinearTol ) THEN  ! NO
        Converged = .TRUE.
        EXIT
     ELSE ! YES
        PrevNorm = Norm
     END IF
!------------------------------------------------------------------
  END DO ! of the nonlinear iteration
!------------------------------------------------------------------
```

After leaving the nonlinear iteration loop the status of convergence shall be displayed on stdio

```
  ! has non-linear solution converged?
  ! -------------------------------
  IF ((.NOT.Converged) .AND. (NonlinearIter > 1)) THEN
     WRITE( Message, * ) 'Nonlinear solution has not converged',&
          'Relative Change=',RelativeChange,'>',NonlinearTol
     CALL Warn('MyHeatSolve', Message)
  ELSE
     WRITE( Message, * ) 'Nonlinear solution has converged after ',&
          iter,' steps.'
     CALL Info('MyHeatSolve',Message,Level=1)
  END IF
```

In the code lines given above, the user could exchange the routine `Warn` by `Fatal` if the simulation should stop upon failed nonlinear iteration convergence.
Further we have to include the needed local subroutines using the Fortran 90 command

```
!------------------------------------------------------------------
! internal subroutines of MyHeatSolver
!------------------------------------------------------------------
CONTAINS
```

The subroutine `LocalMatrix` composes the local matrices and vectors for a bulk element. The header with the variable declaration reads as follows

```
!------------------------------------------------------------------
  SUBROUTINE LocalMatrix(MASS, STIFF, FORCE, LOAD, Element, n, &
       HeatCapacity, HeatConductivity, Density, TransientSimulation)
    IMPLICIT NONE
!------------------------------------------------------------------
    REAL(KIND=dp), DIMENSION(:,:) :: MASS, STIFF
    REAL(KIND=dp), DIMENSION(:) :: FORCE, LOAD, &
         HeatCapacity, HeatConductivity, Density
    INTEGER :: n
    TYPE(Element_t), POINTER :: Element
    LOGICAL :: TransientSimulation
!------------------------------------------------------------------
    REAL(KIND=dp) :: Basis(n),dBasisdx(n,3),ddBasisddx(n,3,3)
    REAL(KIND=dp) :: detJ, LoadAtIP,&
         LocalHeatCapacity, LocalHeatConductivity, LocalDensity
    LOGICAL :: Stat
    INTEGER :: t,i,j,DIM
    TYPE(GaussIntegrationPoints_t) :: IP

    TYPE(Nodes_t) :: Nodes
    SAVE Nodes
```

For the sake of simplicity we use the same identifiers as in the solver subroutine for the variables in the argument list.

The next step is to inquire the dimension of the coordinate system. Thereafter, we get the nodes of the element using the already introduced function `GetElementNodes`. Since the values in `CurrentModel % CurrentElement` and `CurrentModel % Solver` have been set, no additional arguments to the variable `Nodes` have to be set. After we have initialized the local matrix and vector components to zero, the information upon the Gauss-points needed for integration is inquired by the function `GaussPoints`. They returned variable `IP` is of type `GaussIntegrationPoints_t`.

```
    DIM = CoordinateSystemDimension()

    CALL GetElementNodes( Nodes )

    STIFF = 0.0d0
    FORCE = 0.0d0
    MASS = 0.0d0


    !Numerical integration:
    !----------------------
    IP = GaussPoints( Element )
```

The integration over the element is done by summing over all Gauss-points (from 1 to $N_{\mathrm{IP}} \rightarrow$ `IP % n`. The square root of the determinant of the element coordinate system metric tensor $\sqrt{\det(\mathbf{J}^T \cdot \mathbf{J})} \rightarrow$`DetJ` as well as the local basis functions, $\gamma_i \rightarrow$ `Basis`, their derivatives, $\nabla\gamma_i \rightarrow$ `dBasisdx`, are evaluated for every Gauss-point using the function `ElementInfo`. The variable `ddBasisddx` is just passed as a dummy argument, since the last argument, `getSecondDerivatives` is set to `.FALSE.`. The pointer to the element, `Element`, and its nodes, `Nodes` and the local variables of the Gauss-points `IP % U(t)`, `IP % V(t)` and `IP % W(t)`, are needed as input.

```
!-----------------------------------------------------------------
!   Loop over Gauss-points (element Integration)
!-----------------------------------------------------------------
    DO t=1,IP % n
       !Basis function values & derivatives at the integration point:
       !--------------------------------------------------------------
       getSecondDerivatives = .FALSE.
       stat = ElementInfo( Element, Nodes, IP % U(t), IP % V(t), &
            IP % W(t),  detJ, Basis, dBasisdx, ddBasisddx, &
            getSecondDerivatives)
```

Thereafter, the material parameters at the Gauss-points are evaluated, using the basis function. For instance, the local density, $\varrho|_{\mathrm{IP}} \rightarrow$ `LocalDensity` at the Gauss-point is evaluated as follows:

$$\varrho|_{\mathrm{IP}} = \varrho_i\,\gamma_i|_{\mathrm{IP}},$$

with the sum taken over the nodal index i. The load vector $h/(\varrho\, c_p)|_{\mathrm{IP}} \rightarrow$ `LoadAtIP` is evaluated in a similar way.

```
       !Material parameters at integration point:
       !---------------------------------------
       LocalHeatCapacity = SUM( HeatCapacity(1:n) * Basis(1:n) )
       LocalHeatConductivity = SUM( HeatConductivity(1:n) * Basis(1:n) )
       LocalDensity = SUM( Density(1:n) * Basis(1:n) )
       !The source term at the integration point:
       !----------------------------------------
       LoadAtIP = SUM( Basis(1:n) * LOAD(1:n) ) &
            /(LocalHeatCapacity * LocalDensity)
```

The force vector is obtained by the integral over the element, which is approximated by the sum over all Gauss-point contributions

$$F_j = \int\limits_V \frac{h}{\varrho\, c_p}\gamma_j \, DV \approx \sum_{t=1}^{N_{\mathrm{IP}}} \left(\sqrt{ds^2} \sqrt{\det(\mathbf{J}^T \cdot \mathbf{J})} \frac{h}{\varrho\, c_p}\, \gamma_j \right) |_{\mathrm{IP}}.$$

The model coordinate system metric $\sqrt{ds^2}$ $\rightarrow$ `IP % s(t)` as well as the previously inquired element coordinate system metric $\sqrt{\det(\mathbf{J}^T \cdot \mathbf{J})}$ $\rightarrow$ `DetJ` have to be taken into account.
The matrix components are evaluated in complete analogy to the force vector

$$\mathbf{M}_{i\,j} = \int\limits_V \gamma_j \gamma_i \, dV \approx \sum_{t=1}^{N_{\mathrm{IP}}} \left(\sqrt{ds^2} \sqrt{\det(\mathbf{J}^T \cdot \mathbf{J})} \gamma_j \gamma_i \right) |_{\mathrm{IP}},$$

$$\mathbf{A}_{i\,j} = \int\limits_V \frac{k}{c_p\, \varrho} \nabla\gamma_j \cdot \nabla\gamma_i \, dV \approx \sum_{t=1}^{N_{\mathrm{IP}}} \left[\sqrt{ds^2} \sqrt{\det(\mathbf{J}^T \cdot \mathbf{J})} \frac{k}{c_p\, \varrho} \; (\nabla\gamma_j \cdot \nabla\gamma_i) \right] |_{\mathrm{IP}},$$

where the dot product of the first derivatives of the basis function is implemented using the expression $\nabla\gamma_j \cdot \nabla\gamma_i$ $\rightarrow$ `SUM(dBasisdx(i,1:DIM) * dBasisdx(j,1:DIM))`

```
!-----------------------------------------------------------------
!      Loop over j-components of matrices and over force vector
!-----------------------------------------------------------------
       DO j=1,n
          FORCE(j) = FORCE(j) + IP % s(t) * DetJ * LoadAtIP * Basis(j)
!-----------------------------------------------------------------
!         Loop over i-components of matrices
!-----------------------------------------------------------------
          DO i=1,n
             !The mass matrix, if needed
             !-------------------------
             IF (TransientSimulation) THEN
                MASS(i,j) = MASS(i,j)+ IP % s(t) * DetJ * &
                     Basis(i)*Basis(j)
             END IF

             !Finally, the stiffness matrix:
             !-----------------------------
             STIFF(i,j) = STIFF(i,j)  &
                  + IP % s(t) * DetJ * LocalHeatConductivity &
                  * SUM(dBasisdx(i,1:DIM) * dBasisdx(j,1:DIM))&
                  /(LocalDensity * LocalHeatCapacity)
!-----------------------------------------------------------------
          END DO ! end Loop over i-components of matrices
!-----------------------------------------------------------------
```

```
      END DO ! end Loop over j-components of matrices and vector
!-----------------------------------------------------------------
    END DO ! end Loop over Gauss-points (element Integration)
!-----------------------------------------------------------------
  END SUBROUTINE LocalMatrix
!-----------------------------------------------------------------
```

The last two statements in the code sequence given above close the loop over the Gauss-points and provide the end statement of the local subroutine `LocalMatrix`.
The subroutine `BoundaryCondition` evaluates the contribution to the force vector at the boundary elements with given external load $l = q_n/(c_p\,\varrho) \rightarrow$ `LOAD`

$$F_j = \oint_{\partial V} l\,dV \approx \sum_{t=1}^{N_{\mathrm{IP}}} \left(\sqrt{ds^2}\sqrt{\det(\mathbf{J}^T \cdot \mathbf{J})}l \right)|_{\mathrm{IP}}.$$

Since this is implemented in complete analogy to the assembly of the force vector in the previously discussed subroutine `LocalMatrix`, a detailed explanation can be omitted

```
!-----------------------------------------------------------------
  SUBROUTINE BoundaryCondition(LOAD, FORCE, Element, n)
    IMPLICIT NONE
!-----------------------------------------------------------------
    REAL(KIND=dp), DIMENSION(:) :: FORCE, LOAD
    INTEGER :: n
    TYPE(Element_t), POINTER :: Element
!-----------------------------------------------------------------
    REAL(KIND=dp) :: Basis(n),dBasisdx(n,3),ddBasisddx(n,3,3)
    REAL(KIND=dp) :: detJ, LoadAtIP,&
         LocalHeatCapacity, LocalDensity
    LOGICAL :: stat, getSecondDerivatives
    INTEGER :: t,j
    TYPE(GaussIntegrationPoints_t) :: IP

    TYPE(Nodes_t) :: Nodes
    SAVE Nodes
!-----------------------------------------------------------------

    CALL GetElementNodes( Nodes )

    FORCE = 0.0d0

    !Numerical integration:
    !---------------------
    IP = GaussPoints( Element )
!------------------------------------------------------------------
!   Loop over Gauss-points (boundary element Integration)
!------------------------------------------------------------------
    DO t=1,IP % n
       !Basis function values & derivatives at the integration point:
       !--------------------------------------------------------------
       getSecondDerivatives = .FALSE.
       stat = ElementInfo( Element, Nodes, IP % U(t), IP % V(t), &
            IP % W(t),  detJ, Basis, dBasisdx, ddBasisddx, &
            getSecondDerivatives)
       !The source term at the integration point:
```

```
       !---------------------------------------
       LoadAtIP = SUM( Basis(1:n) * LOAD(1:n) )
!-------------------------------------------------------------------
!      Loop over j-components of matrices and over force vector
!-------------------------------------------------------------------
       DO j=1,n
          FORCE(j) = FORCE(j) + IP % s(t) * DetJ * LoadAtIP * Basis(j)
       END DO
    END DO
!------------------------------------------------------------------
  END SUBROUTINE BoundaryCondition
!------------------------------------------------------------------
```

The Fortran 90 file is completed providing the end statement for the user solver subroutine `MyHeatSolver`.

```
!------------------------------------------------------------------
END SUBROUTINE MyHeatSolver
!------------------------------------------------------------------
```

11.5 Compilation and Linking

As already mentioned, the Elmer Solver is written in Fortran 90. The modularity of Elmer implies the use of modules, which are included by the command `USE` in the header of the user functions.

Since these modules are binaries, they in general are incompatible between different compilers on the same platform. This is not an issue on commercial UNIX platforms, such as IRIX (Silicon Graphics) and TRU64 (Alpha Compaq/HP), where the compilers normally are vendor specific. But on Linux as well as Windows, there is more than one Fortran 90 compiler available - for instance the Absoft and Intel compilers on Linux. Hence, if the user wants to include dynamically linked code, it is essential that the same compiler the Elmer Solver source has been compiled with is also used for compilation of the user function.

Let the directory of the installation tree of Elmer be referred to by the system variable `ELMER_HOME` (e.g. `/usr/local/ELMER3.0` on Unix/Linux-systems or `C:\Programs\ELMER3.0` on Windows). The modules that are needed for the compilation are to be found in the subdirectory `include` of the `ELMER_HOME`-tree – `$ELMER_HOME/include` on Unix/Linux systems. The libraries needed for linking are stored in the subdirectory `lib` of the `ELMER_HOME`-tree. Mind, that on Unix/Linux platforms the filename as well as the path are case-sensitive.

11.5.1 IRIX

On an Silicon Graphics IRIX system the subroutine or function in the file `mysolver.f90` is compiled by the command

```
f90 -I$ELMER_HOME/include mysolver.f90 -o mysolver -shared
```

No additional libraries have to be linked to the shared object. The binary in our example is called `mysolver`.

11.5.2 TRU64

The same syntax as for the IRIX compiler applies also to the Compaq Fortran 90 compiler

```
f90 -I$ELMER_HOME/include mysolver.f90 -o mysolver -shared
```

11.5.3 Linux (Intel Fortran)

The 32-bit Linux version of Elmer Solver has been compiled using the Intel Fortran compiler (see details under `http://www.intel.com/software/products/compilers/flin/`). The compiler call is `ifc`. From the compiler side in order to obtain a working executable the library `libimf.so` has to be linked. If the variable `IFC_HOME` contains the path to the installation directory of the compiler (e.g., `IFC_HOME = /opt/intel/compiler70` for version 7.0), this library is then to be found under `$IFC_HOME/libimf.so`.

On an Intel Pentium IV using RedHat Linux version 9 the following line (given in one line at the command prompt) compiles the user file `mysolver.f90` containing the Fortran 90 code for a user subroutine or user function and links it to the Elmer Solver library, `$ELMER_HOME/lib/libSolver.so`, and the earlier mentioned compiler specific library. The final executable is stored in the file `mysolver`:

```
ifc -xW -tpp7 -vec_report0 -w -O -I$ELMER_HOME/include -o mysolver
    mysolver.f90 -shared -L/$ELMER_HOME/lib -L$IFC_HOME/ia32/lib
    -lSolver -limf
```

The options `-xW` and `-tpp7` are for special optimization of the code for the Pentium IV architecture and have to be replaced or omitted if compiling on another hardware platform. `-w` switches off warnings and `-O` sets the lowest level of compiler optimization – higher orders usually tend to cause problems and should be used with care. The `-I` indicates the include directory for modules, whereas the directories after the `-L` contain the libraries that are linked to the compiled object. Mind, that these library-paths always have to be added at the very end of the command line. The `-shared` option takes care that dynamically linked libraries are used.

11.5.4 Windows

The Windows version of Elmer Solver has been compiled using the DECWindows Fortran compiler. The subroutine `mysolver.f90` is compiled from the command line entering

```
f90 -I%ELMER_HOME%\include -dll mysolver.f90 %ELMER_HOME%\Solver.lib
```

It is important that the keyword `DLLEXPORT` followed by the name of the subroutine is inserted immediately after the interface of the subroutine. In the case of the example given in 11.4.2, this would look as follows

```
SUBROUTINE MyHeatSolver( Model,Solver,dt,TransientSimulation )
DLLEXPORT MyHeatSolver
...
```

After successful compilation, the file `mysolver.dll` is to be found in the local directory. In the filename declaration of the `Procedure`-keyword in solver input file, the suffix `.dll` can be omitted

```
Solver 1
  Procedure = "mysolver" "subroutineName"
  ...
End
```

Appendix A

Format of mesh files

In this appendix the format of ElmerSolver mesh files is desribed. The mesh data are arranged into four separate files: `mesh.header`, `mesh.nodes`, `mesh.elements`, and `mesh.boundary`. Here the contents of these files will be described.

In the mesh files numeric codes are used for distinguishing different element types. For the element type codes and the node numbering order of the elements see also appendix D.

A.1 The format of header file

The header file `mesh.header` tells how many nodes and elements are present in the mesh. The lines of this file are organized as

```
nodes elements boundary-elements
nof_types
type-code nof_elements
type-code nof_elements
...
```

In the first line the numbers of nodes, elements, and boundary elements are given, while the count in the second line is the number of different element types used in the mesh. The lines which follow give the numbers of elements as sorted into different element types.

For example, the following header file

```
300 261 76
2
404 261
202 76
```

tells us that the mesh is composed of 300 nodes, 261 elements, and 76 boundary elements. Two different element types are used in the mesh: there are 261 elements of type code 404 (bilinear quadrilateral) and 76 elements of type code 202 (linear line element).

A.2 The format of node file

The file `mesh.nodes` contains node data so that each line defines one node. Each line starts with two integers followed by three real numbers:

```
n1 p x y z
n2 p x y z
 ...
nn p x y z
```

The first integer is the identification number for the node. The second integer is a partition index for parallel execution and is not usually referenced by the solver in the case of sequential runs. If the partition index is not of particular use, it may be set to be -1 (or 1). The real numbers are the spatial coordinates of the node. Three coordinates should always be given, even if the simulation was done in 1D or 2D. It is also noted that the nodes may be listed in any order.

A.3 The format of element file

The `mesh.elements` file contains element data arranged as

```
e1 body type n1 ... nn
e2 body type n1 ... nn
...
en body type n1 ... nn
```

Each line starts with an integer which is used for identifying the element. The integer `body` defines the material body which this element is part of. Then the element type code and element nodes are listed. For example, the element file might start with the following lines:

```
1 1 404 1 2 32 31
2 1 404 2 3 33 32
3 1 404 3 4 34 33
4 1 404 4 5 35 34
...
```

A.4 The format of boundary element file

The elements that form the boundary are listed in the file `mesh.boundary`. This file is similar to the `mesh.elements` file and is organized as

```
e1 bndry p1 p2 type n1 ... nn
e2 bndry p1 p2 type n1 ... nn
...
en bndry p1 p2 type n1 ... nn
```

The first integer is again the identification number of the boundary element. Next the identification number of the part of the boundary where this element is located is given. Whether the boundary element can be represented as the side of a parent element defined in the file `mesh.elements` is indicated using the two parent element numbers `p1` and `p2`. If the boundary element is located on an outer boundary of the body, it has only one parent element and either of these two integers may be set to be zero. It is also possible that both parent element numbers are zeros. Finally the element type code and element nodes are listed.

Appendix B

Format of result output files

B.1 Format versions

Result files can be written as either ASCII text or in binary. This is controlled by the parameter

```
   Binary output = logical true|false
```

in the 'Simulation' section of the .sif file. Default is `false`.

The format of the file is recorded on it's first line;[1] it's either

`BINARY` $v.e$

or

`ASCII` v

The v at denotes the version number of the format, and the e in the binary format denotes an endianess-marker; either `L` for little endian or `B` for big endian.

ElmerSolver can read files of older format versions for restarting, but all new files are written in the newest formats. The current formats documented here are ASCII version 1 and BINARY version 2.

B.2 General structure

Both binary and ASCII files have the following general structure. In the binary files, the header is separated from the rest by a null byte. The ASCII format has no such separator.

```
[File format version line]
[Header]
[<null byte> (binary only)]
[timestep 1]
[timestep 2]
[timestep 3]
   .
   .
   .
[timestep n]
```

[1]except for old ASCII files, that lack the format version line, and start with "`!File started at:`"

B.2.1 The header

The header looks the same for both binary and ASCII (ans is written in ASCII also for binary files):

```
!File started at: date time
 Degrees of freedom:
 variable 1       n1  :fs
 variable 2       n2  :fs
 variable 3       n3  :fs
           .
           .
           .
 Total DOFs:       nTotDOFs
 Number Of Nodes:       nNodes
```

Note that in the list of variables, vectors appear both as vectors (DOF > 1) and separate components (DOF = 1).

B.2.2 Timesteps

For each time step, the time and the values of the variables are stored. For vector variables, the components are stored as separate variables, typically named *varname 1*, *varname 2*, etc.

If the parameter

```
Omit unchanged variables in output = logical true|false
```

in the 'Simulation' section of the .sif file is set to `true`, only variables whose values has changes since last time are saved. Default is `false`

For the binary format, the following type specifiers are used in this document:

<s(str)>	Null terminated string of characters.
<i(i4)>	4 byte integer.
<j(i8)>	8 byte integer.
<x(dbl)>	8 byte floating point number.

For this part of the file, the general structure of binary and ASCII files are essantially the same, with just some minor differences:

ASCII	Binary	
`Time:` ns nt t	<`Time:`(`str`)><ns(`i4`)><nt(`i4`)><t(`dbl`)>	
Variablename_1	<*Variablename_1*(`str`)>	
`[Permutation table` p_1`]`	`[Permutation table` p_1`]`	
$\vdots$	$\vdots$	
$Var_1(p_1(i))$	$<Var_1(p_1(i))$(`dbl`)>	Variable 1's values $\forall\, i$ s.t. $p_1(i) > 0$.
$\vdots$	$\vdots$	
Variablename_2	<*Variablename_2*(`str`)>	
`[Permutation table` p_2`]`	`[Permutation table` p_2`]`	
$\vdots$	$\vdots$	
$Var_2(p_2(i))$	$<Var_2(p_2(i))$(`dbl`)>	Variable 2's values $\forall\, i$ s.t. $p_2(i) > 0$.
$\vdots$	$\vdots$	
Variablename_3	<*Variablename_3*(`str`)>	
`[Permutation table` p_3`]`	`[Permutation table` p_3`]`	
$\vdots$	$\vdots$	
$\vdots$	$\vdots$	
$Var_3(p_3(i))$	$<Var_3(p_3(i))$(`dbl`)>	Variable 3's values $\forall\, i$ s.t. $p_3(i) > 0$.
$\vdots$	$\vdots$	

nt= time step number, ns= saved time steps number, t= time.

The permutation tables

The permutation tables can be stored in three different ways:

1. As an explicit table:

ASCII	Binary	
Perm: $size$ np	<$size$(`i4`)><np(`i4`)>	
$\vdots$	$\vdots$	
i $p(i)$	<i(`i4`)><$p(i)$(`i4`)>	Permutation indexes i and values $p(i)$ $\forall\, i$ s.t. $p(i) > 0$.
$\vdots$	$\vdots$	

$size$ = total size of the permutation table (> 0), and np = number of positive values in the table.

2. If the permutation table is the same as for the previous variable, there's no need to store it again. This case is written as

ASCII	Binary
`Perm:  use previous`	<-1(`i4`)><Pos(`i8`)>

Pos in the binary format is the position in bytes of the previous table.

3. No permutation table; corresponds to the case

$$size = np = nNodes, \text{ and } p(i) = i \quad \forall\, i.$$

This case is stored as

ASCII	Binary
`Perm:  NULL`	<0(`i4`)>

B.3 The positions file

For binary format, a positions file named ’*outputfile*.pos’ will be created. It contains the positions (in bytes) of the timesteps and variables in the result file, expressed as 8 byte integers. It has the following format ($nVar$ = number of variables):

<Endianess-marker `(char)`>
<$nVar$`(i4)`>
<varname 1`(str)`>
<varname 2`(str)`>
$\vdots$
<varname nVar`(str)`>
<Pos. for Timestep 1`(i8)`>
<Pos. for variable 1`(i8)`>
<Pos. for variable 2`(i8)`>
$\vdots$
<Pos. for variable $nVar$`(i8)`>
<Pos. for Timestep 2`(i8)`>
<Pos. for variable 1`(i8)`>
<Pos. for variable 2`(i8)`>
$\vdots$
<Pos. for variable $nVar$`(i8)`>
<Pos. for Timestep 3`(i8)`>
<Pos. for variable 1`(i8)`>
<Pos. for variable 2`(i8)`>
$\vdots$
<Pos. for variable $nVar$`(i8)`>
$\vdots$

Note: Positions are saved for *all* variables for every time step; even if an unchanged variable isn’t saved to the result file for a time step, it will still have a position in the .pos file (i.e. the position of where it was saved last time). Because of this all timesteps has the same size of $(nVar+1)\times 8$ bytes. Finding the position of the n:th variable of the m:th time step is therefore easy; it’s found at the

$$(\textit{size-of-header} + ((nVar+1)\times(m-1)+n)\times 8) : \text{th}$$

byte in the positions file.

Appendix C

Format of ElmerPost Input File

The lines of ElmerPost input file are organized as

```
nn ne nf nt scalar: name vector: name ...
x0 y0 z0
...        ! nn rows of node coordinates (x,y,z)
xn yn zn
group-name element-type i0 ... in
...        ! group data and element decriptions
group-name element-type i0 ... in
#time 1 timestep1 time1
vx vy vz p ...
...        ! nn rows
vx vy vz p ...
#time 2 timestep2 time2
vx vy vz p
...        ! nn rows
vx vy vz p ...
 ....
#time n timestepn timen
vx vy vz p ...
...        ! nn rows
vx vy vz p ...
```

The header

The file starts with the header line which contains the following information:

- `nn`: the total number of nodes
- `ne`: the total number of the elements including boundary elements
- `nf`: the total number of degrees of freedom, i.e. the total number of scalar unknowns in the model
- `nt`: the number of time steps for which solution data is stored
- `scalar: name vector: name ...` : the list which pairs variable names with their types.

The mesh and group data

After the header the node coordinates are given, each coordinate triplet on its own row. Three coordinates shoud be given even if the model was two-dimensional.

Group data consist of the following information:

- `group-name`: the name of the element group (having the same material, body etc.)
- `element-type`: the numeric code giving the element type; see also Appendix D.
- The numbers `i0 ... in` are the indeces of the element nodes. The nodes are referenced using the row indeces of the node coordinate array at the beginning of the file The first node in the array has the index zero.

It is noted that there is also another level of element grouping that can be employed as follows

```
#group group1
  element-definitions
        ...
#group group2
  element-definitions
        ...
#endgroup group2
  element-definitions
        ...
#endgroup group1
```

The number of element groups is not restricted in any way.

The solution data

For each timestep the following solution data is written:

- `#time n t time`: `n` is the order number of the solution data set, `t` is the simulation timestep number, and `time` is the current simulation time.
- The next `nn` rows give the node values of the degrees of freedom. The values are listed in the same order as given in the header with the keywords `scalar:` and `vector:`

An example file

Here a very simple example file is given. There is only one element, three nodes, one variable, and the solution data are given for a single timestep:

```
3 1 1 1 scalar: Temperature
0 0 0
1 0 0
0 1 0
#group all
body1 303 0 1 2
#endgroup all
#time 1 1 0
1
2
3
```

Appendix D

Basic element types

The basic element types which ElmerSolver can handle are the linear and quadratic elements in one, two, and three dimensions:

- linear (element type code 202) and quadratic (203) elements in one dimension
- linear (303) and quadratic (306) triangles with three and six nodes, respectively; see Figure D.1

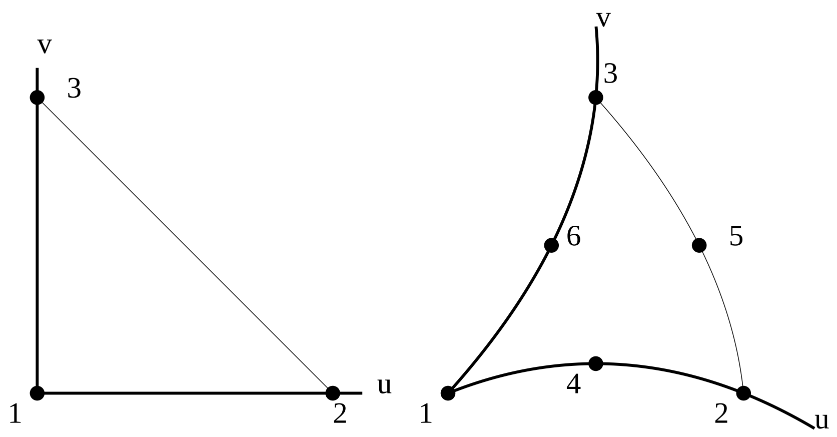


Figure D.1: The linear (303) and quadratic (306) triangular elements.

- bilinear (404) and quadratic (408,409) quadrilaterals with four, eight, and nine nodes, respectively; see Figure D.2
- linear (504) and quadratic (510) tetrahedrons with four and ten nodes, respectively; see Figure D.3
- trilinear (808) and quadratic (820,827) bricks with 8, 20, and 27 nodal points, respectively; see Figure D.4.

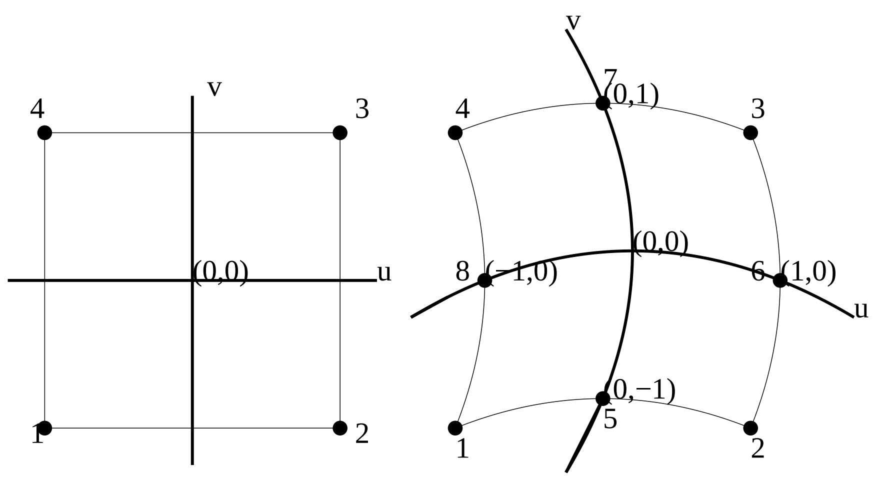


Figure D.2: The four-node (404) and eight-node (408) quadrilateral elements.

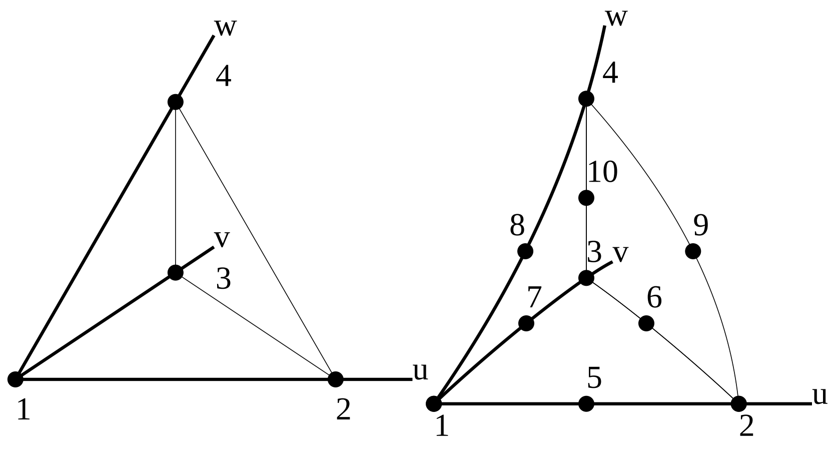


Figure D.3: The linear (504) and quadratic (510) tetrahedron elements.

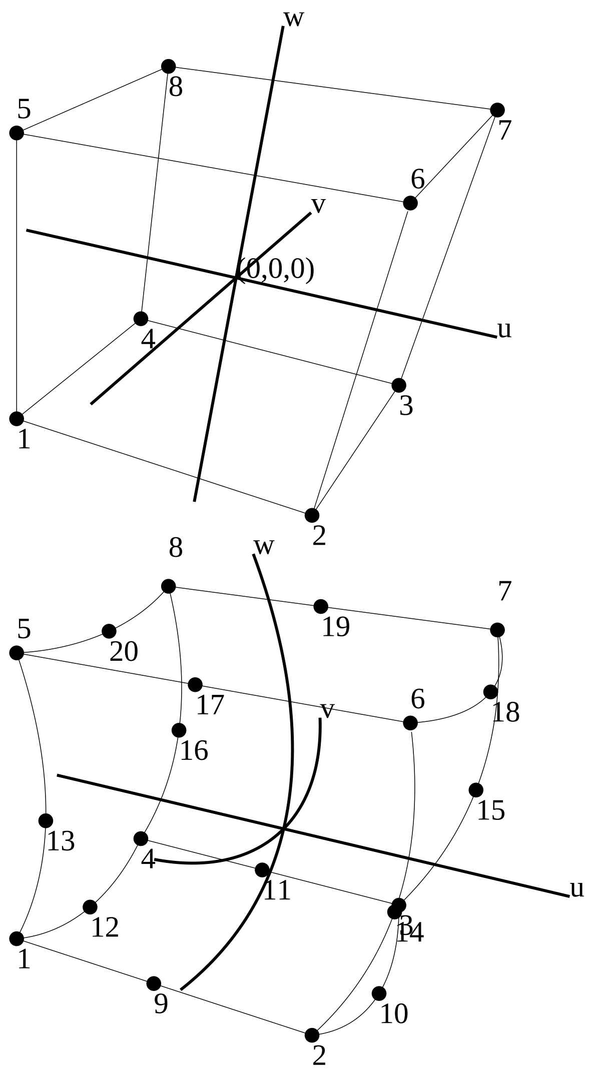


Figure D.4: The 8-node (808) and 20-node (820) brick elements.

Appendix E

Higher-order finite elements

E.1 Theory

Higher-order finite elements are elements for which the degree of basis functions is higher than 1. They differ from usual Lagrange -type elements in a sense that in addition to nodal basis functions there exists basis functions, which are associated with edges, faces and interiors of elements.

- **Size modes** get their values along some edge of element. They vanish towards other edges and all nodal points of element. Side modes are defined for all 2d and 3d elements.
- **Face modes** get their values along some face of element. They vanish towards other faces and all edges and nodal points of element. Face modes are only defined for 3d elements.
- **Internal modes** get their values inside element and vanish towards elements faces, edges and nodal points. They are defined for all 1d, 2d and 3d elements.

Higher-order elements are usually also called p -elements. Properties for good p-elements include computational efficiency, at least partial orthogonality and hierarchy of basis functions. With hierarchy we mean that if basis for some element of some given degree p is $\mathcal{B}^p$ for $p+1$ it holds that $\mathcal{B}^p \subset \mathcal{B}^{p+1}$. Orthogonal properties of basis functions ensure, that condition number of the global stiffness matrix does not increase as dramatically as for nodal (Lagrange) elements of higher order. This ensures good numerical stability. Some good references to higher-order finite elements in literature are [3] by Szabo and Babuska and [4] by Solin et al.

The usual element interpolant, now denoted as $u_{h,p}$, is for p elements the sum of nodal, edge, face and bubble interpolants

$$u_{h,p} = u^v_{h,p} + u^e_{h,p} + u^f_{h,p} + u^b_{h,p} \tag{E.1}$$

where $u^v_{h,p}$ is nodal interpolant as defined before and $u^e_{h,p}$ edge, $u^f_{h,p}$ face and $u^b_{h,p}$ bubble interpolants. Let n_e be the number of edges and n_f number of faces in an element. Edge and face interpolants are defined as

$$\begin{aligned} u^e_{h,p} &= \sum_{i=1}^{n_e} u^{e_i}_{h,p} \\ u^f_{h,p} &= \sum_{i=1}^{n_f} u^{f_i}_{h,p} \end{aligned}$$

Contribution of one p -element to global system is equivalent to that of h-element. Naturally for higher-order elements the number of local stiffness matrix elements to contribute to global system is greater, because of the larger number of basis functions.

Generally using p -elements yields a better approximation than using normal linear elements. In fact, convergence for p elements is exponential when there are no singularities inside or on the boundary of the solution domain. When there are singular points inside the domain convergence is algebraic. If singular point is a nodal point convergence is twice that of h-method, otherwise it is equal to the h-method.

E.2 Higher-order elements in Elmer

Elements implemented in Elmer follow the ones presented in [3]. Now let us define some orthogonal polynomials based on Legendre polynomials $P_i(x), i \geq 0$. So called lobatto shape functions ϕ_k are defined as

$$\phi_k(\xi) = \sqrt{\frac{1}{2(2k-1)}}(P_k(\xi) - P_{k-2}(\xi)),\ k = 2, 3, \ldots \tag{E.2}$$

where P_k are Legendre polynomials. Function ϕ has two of its roots at ± 1, so now define another function, φ_i as

$$\varphi_k(\xi) = \frac{4\phi_k(\xi)}{1-\xi^2},\ k = 2, \ldots, p \tag{E.3}$$

Functions ϕ_i and φ_i are used to define higher order elements. Different element shapes and their their basis functions are defined in appendix E.4. Pyramidal element used in Elmer is based loosely to Devloos representation in [2].

In Elmer elements with varying polynomial degree p may be used in the same mesh. It is also possible to combine elements of different types in the same mesh, as defined basis functions for edges and faces for different element types are compatible with one another. Pyramidal and wedge higher-order elements to connect tetrahedral and brick elements are also supported. To achieve best possible converge the use of pyramidal elements in a mesh should be kept to a minimum. Global continuity of higher order finite element space used is enforced by the solver, when method `ElementInfo` is used for obtaining basis functions values for elements.

To combine elements of varying degree in mesh maximum rule is used. Thus if two or more elements share an edge and have differing polynomial degrees, maximum of edge's degrees is choosed as degree of global edge.

To declare polynomial degree greater than one to an element, element definition in `mesh.elements` -file needs to be changed. For p -elements, element definition syntax is

$$T_e[\text{p}p_e]$$

where $T_e = \{202, 303, 404, 504, 605, 706, 808\}$ is the element type and $p_e \geq 1$ polynomial degree of element. Setting $p_e = 0$ equals using normal linear basis defined in Elmer. For example, a triangle with polymial degree 4 could be defined in mesh.elements file as follows

$$303\text{p}4$$

The actual number of degrees of freedom for edges, faces or bubbles of element types is defined by element polynomial degree p. Each degree of freedom in element is associated with some basis function. The following table gives the number of degrees of freedom for elements used in Elmer.

Element	Nodes	Edges	Faces	Bubbles
Line	2	-	-	$p-1$
Quadrilateral	4	$4(p-1)$	-	$\frac{(p-2)(p-3)}{2}$
Triangle	3	$3(p-1)$	-	$\frac{(p-1)(p-2)}{2}$
Brick	8	$12(p-1)$	$3(p-2)(p-3)$	$\frac{(p-3)(p-4)(p-5)}{6}$
Tetrahedron	4	$6(p-1)$	$2(p-1)(p-2)$	$\frac{(p-1)(p-2)(p-3)}{6}$
Wedge	6	$9(p-1)$	-	$\frac{(p-2)(p-3)(p-4)}{6}$
(quad. face)	-	-	$\frac{3(p-2)(p-3)}{2}$	-
(triang. face)	-	-	$(p-1)(p-2)$	-
Pyramidi	5	$8(p-1)$	-	$\frac{(p-1)(p-2)(p-3)}{6}$
(quad. face)	-	-	$\frac{(p-2)(p-3)}{2}$	-
(triang. face)	-	-	$2(p-1)(p-2)$	-

It is worth noting, however, that used Solver (HeatSolve, StressSolve, etc.) used must be modified to support elements of higher degree. Usually this only consists of making local stiffness matrix and force vector larger.

A p-element passed to Elmer gaussian point generator `GaussPoints` defined in module `Integration` returns enough integration points to integrate worst case product of two element basis functions. Here worst case is integration over two basis functions for which $p_m = \max\{p_e, p_f, p_b\}$. As gaussian quadrature is accurate to degree $p = 2n - 1$, where n is the number of points used, number of points for each element is calculated from

$$n = \frac{2p_m + 1}{2} \tag{E.4}$$

and rounded up to nearest integer. To get the final number of points for multiple integrals, n is raised to the power of element dimension. If integral includes a non-constant factor, i.e $\int_K \alpha\phi_i\phi_j$ where α is a function of degree k, numerical integration is not accurate and number of integration points needs to be set manually. Now minimum number of gaussian points to integrate element accurately becomes

$$n = \frac{\min\{2p_m + k, 3p_m\} + 1}{2} \tag{E.5}$$

which may again be rounded up to nearest integer and raised to power of element dimension to get the actual number of integration points.

E.2.1 Boundary conditions

Boundary elements (elements, which lie on a boundary of a computational domain) obey the parity of their parent element. Basis for elements on boundary is defined so that it represents a projection from high to low dimension in element space. Thus it is possible to integrate along the boundary of the computational domain and use values obtained to set Neumann boundary conditions, for example. Treatment of Neumann and Newtonian is analogous to classical cases presented in many finite element method textbooks, except for the greater number of basis functions to set.

In Elmer, Newtonial and Neumann boundary conditions are set by integrating over element boundaries and contributing these integrals to global system. For higher order elements this procedure may also be used, because higher order functions of boundary elements are given the direction of their parent. Thus values returned for boundary element are equal to values of their parent elements higher order functions on element boundary. Indexes for contribution to global system may be acquired from procedure defined in module `DefUtils`

```
getBoundaryIndexes( Mesh, Element, Parent, Indexes, indSize )
```

which returns global indexes of contribution for boundary element `Element` to given vector `Indexes`, given the finite element mesh `Mesh` and parent element `Parent` of boundary element. Also the size of created index vector is returned to `indSize`.

Nonhomogeneous Dirichlet type boundary conditions, e.g. $u = g$, on ∂T are more difficult to handle for higher order elements. Even though the nodal values are known, the coefficients of higher order functions are linear combinations over whole element boundary and thus it cannot be set as a nodal value.

Subroutine `DefaultDirichletBCs` solves unknown coefficients of higher order functions by minimizing boundary problem energy. Problem given is then equivalent to that of standard fem, except that integrals and functions are calculated along boundary of the computational domain. Generally, from a solver user point of view, Dirichlet boundary conditions need no extra actions compared to the use of normal elements.

E.2.2 Some practical aspects

Typical singular points in the solution are points where boundary condition or material parameters change abruptly or vertex type singularities (such as the inner node of a l-shaped beam or a crack tip). In these cases convergence of the p-method is twice that of h-method.

However, it is much more expensive computationally to use high polynomial degree than use many elements of low degree. Therefore, if possible, mesh should be designed in a way that near nodal singularities small low degree ($p = 1$) elements were used. In other parts of the solution domain, where the solution is smoother, large elements with high polynomial degree are adviced. As Elmer is not hp-adaptive, and element polynomial degree is not modified by the solver, mesh design issues must be taken into account for computational efficiency.

It is well known that for linear problems it is possible reduce the size of the global problem by leaving out all bubble functions. This procedure is often called condensation. In Elmer condensation for local stiffness matrix may be done (and is adviced to be done) for linear systems which do not need stabilization. Condensation is done by routine `CondensateP` located in module `SolverUtils`. More precisely routine is expressed as

```
CondensateP(N, Nb, K, F, F1)
```

where `N` is the number of all nodal, edge and face degrees of freedom, `Nb` the number of internal degrees of freedom, `K` local stiffness matrix, `F` local force vector and `F1` optional second force vector.

E.3 ElmerSolver services for higher-order elements

This section describes some of the services related to p elements, which are included in different parts of the Solver.

E.3.1 Properties of p element

For determining p element properties there are several utilities. First of all it is possible to check if some element is a p element by checking elements `isPElement` flag. If flag is set to true, element is a p-element. Functions

```
isPTriangle( Element )
isPTetra( Element )
isPPyramid( Element )
isPWedge( Element )
```

check if given element is p type triangle, tetrahedron, pyramid or wedge. They are implemented because used p reference triangles, tetrahedrals, pyramids and wedges are different than those defined for Lagrange type elements. For determining maximum degrees of element edges or faces, routines

```
getEdgeP( Element, Mesh )
getFaceP( Element, Mesh )
```

return the maximum polynomial degree of elements edges or faces, when given `Element` and finite element mesh `Mesh`.

E.3.2 Fields related to p elements

In module `Types`, type `Element_t` has following p element related fields

```
INTEGER :: TetraType
LOGICAL :: isPElement
LOGICAL :: isEdge
INTEGER :: localNumber
INTEGER :: GaussPoints
```

`Tetratype` defines type of tetrahedral p element. For nontetrahedral elements `Tetratype=0`, for tetrahedral elements `Tetratype=`$\{1, 2\}$.

`isPElement` defines if an element is of higher-order. `isPElement=.TRUE.` for p-elements, `.FALSE.` otherwise.

`isEdge` defines if an element is edge element for some higher entity, i.e. edge or face of a 2d or 3d element. If `isEdge=.TRUE.` element is an edge, `.FALSE.` otherwise.

`localNumber` defines the local number of boundary elements, that is which local edge or face number boundary element has in respect to its' parent element.

`GaussPoints` defines the number of gauss points for element. Value is calculated from $n = (\frac{2p_m+1}{2})^d$, where d is element dimension and p_m element maximum polynomial degree. n is rounded up to nearest integer. Variable `GaussPoints` has enough quadrature points to integrate function of degree $2p_m$ accurately.

When modifying local solver to support higher order elements, the maximum size for some element stiffness matrix or force vector may be obtained from mesh variable `MaxElementDOFs`. This variable is set by the mesh read-in process to the maximum degrees of freedom for single element in mesh.

E.3.3 Higher order basis and element mappings

Basis for higher order elements is defined in module `PElementBase`. Module contains also definitions for ϕ and φ -functions and Legendre polynomials. These definitions have been generated to implicit form with symbolic program **Maple** [1] up to $p_{\max} \leq 20$. This mean that no recursion is needed for generation of values of Legendre polynomials or other lower level components based on them, if used $p < p_{\max}$.

Generally higher order basis functions take as their arguments the point in which to calculate function value and indexing i,$m(i, j)$ or $m(i, j, k)$ depending on the function type. All edge functions take in addition to these parameters a special optional flag, namely `invertEdge`, which defines if direction of edge basis function needs to be inverted. In Elmer all edges are globally traversed from smaller to higher node. That is, let A and B be global node numbers of edges. The varying parameter of edge function then varies between $[-1, 1]$ from $A \rightarrow B$ globalle. Inversion is then used for enforcing global continuity of edge basis functions which are not properly aligned. Edge rule is presented in figure E.3.3

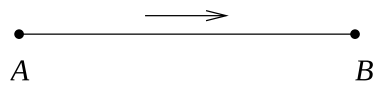


Figure E.1: Global direction of edge. For global node indexes $A < B$

Most of the face functions take as their optional argument the local numbering based on which face functions are formed. This local direction is formed according to global numbers of face nodes. There are rules for triangular and square faces. Let A, B, C be global nodes of a triangular face. Globally face is aligned so that $A < B < C$. For square faces $A = \min\{v_i\}$ where v_i are global nodes of square face and B, C are nodes next to node A on face. Square face is aligned by rule $A < B < C$ for these nodes. These rules are presented in figure E.3.3.

Tetrahedral element is an exception to the above interface rules, i.e. edge and face functions of tetrahedral elements take type of tetrahedral element as their optional argument. This is due to fact that it is possible to reduce any tetrahedral element to one of the two reference tetrahedral elements for which all edges and faces are defined so that their local orientation matches global orientation. This means, that for tetrahedral

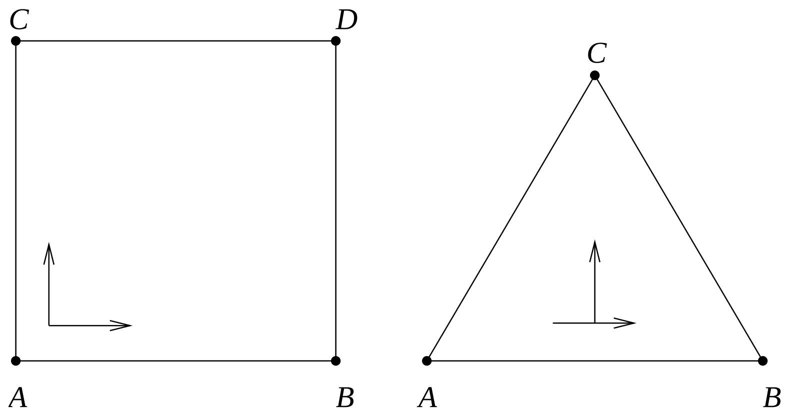


Figure E.2: Global direction of triangular and quadrilateral faces. For global node indexes $A < B < C$; A has lowest index among indexes of face.

elements, global continuity does not need to be enforced, if proper reduction to one of the two reference elements has been made.

Mappings from element nodal numbers to different p element edges or faces are defined in module `PElementMaps`. Mappings generally define which nodes of element belong to certain local edge or face of elements. Mappings to elements edges, faces and from faces to local edge numbers may be obtained from routines `GetElementEdgeMap`, `GetElementFaceMap` and `GetElementFaceEdgeMap`. Mappings may also be accessed by via methods `get`$T_e P_e$`Map`, where T_e is element name and $P_e = \{\text{Edge,Face}\}$ is part of element to get map for. Routine `getElementBoundaryMap` returns mappings for element boundaries depending on element type.

For example, to get global nodes for brick face number 4, one would use the following `Fortran90` code

```
map(1:4) = getBrickFaceMap(4)
nodes(1:4) = Element % NodeIndexes(map)
```

E.4 Higher-order elements

Let $\lambda_1, \lambda_2, \lambda_3 \in \{\pm\xi, \pm\eta, \pm\zeta\}$ and additionally $\bigcap_i \lambda_i = \phi$.

E.5 Line

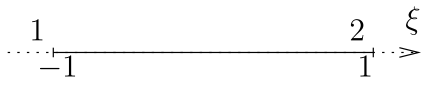


Figure E.3: Line element

E.5.1 Nodal basis

$$L_1 = \frac{1-\xi}{2}$$
$$L_2 = \frac{1+\xi}{2}$$

E.5.2 Bubble basis

$$L_i^{(0)} = \phi_i(\xi),\ i = 2,\ldots,p$$

E.6 Quadrilateral

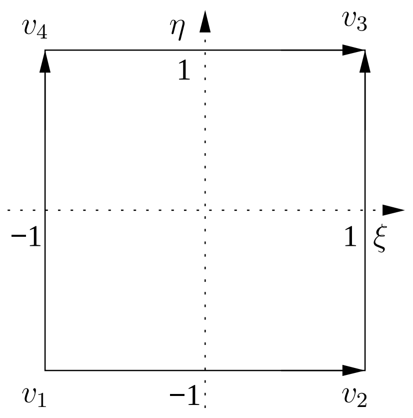


Figure E.4: Quadrilateral element

E.6.1 Nodal basis

$$\begin{aligned}
N_1 &= \frac{1}{4}(1-\xi)(1-\eta) \\
N_2 &= \frac{1}{4}(1+\xi)(1-\eta) \\
N_3 &= \frac{1}{4}(1+\xi)(1+\eta) \\
N_4 &= \frac{1}{4}(1-\xi)(1+\eta)
\end{aligned}$$

E.6.2 Edge basis

$$\begin{aligned}
N_i^{(1,2)} &= \frac{1}{2}(1-\eta)\phi_i(\xi),\ i = 2,\ldots,p \\
N_i^{(2,3)} &= \frac{1}{2}(1+\xi)\phi_i(\eta),\ i = 2,\ldots,p \\
N_i^{(4,3)} &= \frac{1}{2}(1+\eta)\phi_i(\xi),\ i = 2,\ldots,p \\
N_i^{(1,4)} &= \frac{1}{2}(1-\xi)\phi_i(\eta),\ i = 2,\ldots,p
\end{aligned}$$

E.6.3 Bubble basis

$$N_{m(i,j)}^{(0)} = \phi_i(\xi)\phi_j(\eta)$$

where $i,j \geq 2,\ i+j = 4,\ldots,p$

E.7 Triangle

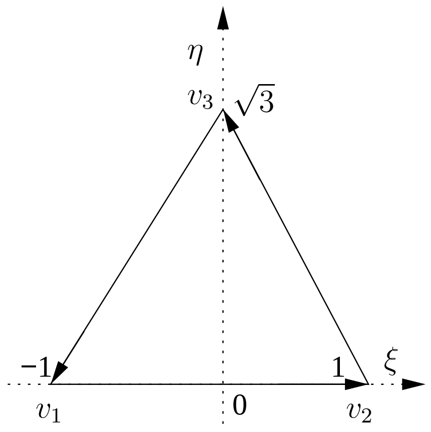


Figure E.5: Triangle element

E.7.1 Nodal basis

$$\begin{aligned} L_1 &= \frac{1}{2}(1 - \xi - \frac{1}{\sqrt{3}}\eta) \\ L_2 &= \frac{1}{2}(1 + \xi - \frac{1}{\sqrt{3}}\eta) \\ L_3 &= \frac{\eta}{\sqrt{3}} \end{aligned}$$

E.7.2 Edge basis

$$\begin{aligned} N_i^{(1,2)} &= L_1 L_2 \varphi_i(L_2 - L_1),\ i = 2, \ldots, p \\ N_i^{(2,3)} &= L_2 L_3 \varphi_i(L_3 - L_2),\ i = 2, \ldots, p \\ N_i^{(3,1)} &= L_3 L_1 \varphi_i(L_1 - L_3),\ i = 2, \ldots, p \end{aligned}$$

E.7.3 Bubble basis

$$N_{m(j,n)}^{(0)} = L_1 L_2 L_3 P_1(L_2 - L_1)^j P_1(2L_3 - 1)^n$$

where $j, n = 0, \ldots, i-3$, $j + n = i - 3,\ i = 3, \ldots, p$

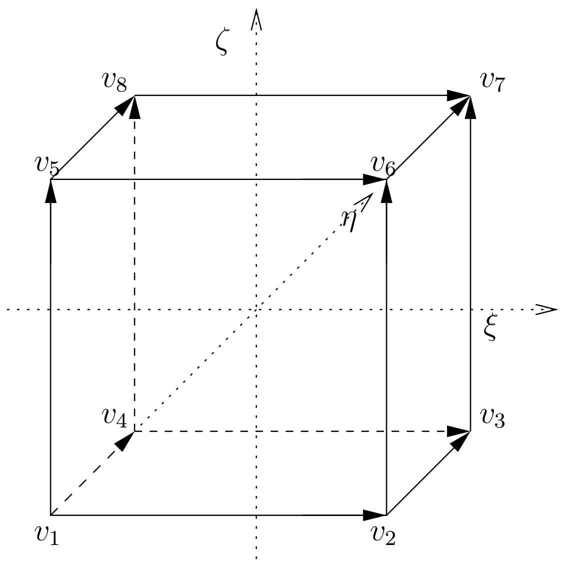


Figure E.6: Brick element

E.8 Brick

E.8.1 Nodal basis

$$\begin{aligned}
N_1 &= \frac{1}{8}(1-\xi)(1-\eta)(1-\zeta) \\
N_2 &= \frac{1}{8}(1+\xi)(1-\eta)(1-\zeta) \\
N_3 &= \frac{1}{8}(1+\xi)(1+\eta)(1-\zeta) \\
N_4 &= \frac{1}{8}(1-\xi)(1+\eta)(1-\zeta) \\
N_5 &= \frac{1}{8}(1-\xi)(1-\eta)(1+\zeta) \\
N_6 &= \frac{1}{8}(1+\xi)(1-\eta)(1+\zeta) \\
N_7 &= \frac{1}{8}(1+\xi)(1+\eta)(1+\zeta) \\
N_8 &= \frac{1}{8}(1-\xi)(1+\eta)(1+\zeta)
\end{aligned}$$

E.8.2 Edge basis

$$
\begin{aligned}
N_{i-1}^{1,2} &= \frac{1}{4}\phi_i(\xi)(1-\eta)(1-\zeta)\\
N_{i-1}^{2,3} &= \frac{1}{4}\phi_i(\eta)(1+\xi)(1-\zeta)\\
N_{i-1}^{4,3} &= \frac{1}{4}\phi_i(\xi)(1+\eta)(1-\zeta)\\
N_{i-1}^{1,4} &= \frac{1}{4}\phi_i(\eta)(1-\xi)(1-\zeta)\\
N_{i-1}^{1,5} &= \frac{1}{4}\phi_i(\zeta)(1-\xi)(1-\eta)\\
N_{i-1}^{2,6} &= \frac{1}{4}\phi_i(\zeta)(1+\xi)(1-\eta)\\
N_{i-1}^{3,7} &= \frac{1}{4}\phi_i(\zeta)(1+\xi)(1+\eta)\\
N_{i-1}^{4,8} &= \frac{1}{4}\phi_i(\zeta)(1-\xi)(1+\eta)\\
N_{i-1}^{5,6} &= \frac{1}{4}\phi_i(\xi)(1-\eta)(1+\zeta)\\
N_{i-1}^{6,7} &= \frac{1}{4}\phi_i(\eta)(1+\xi)(1+\zeta)\\
N_{i-1}^{8,7} &= \frac{1}{4}\phi_i(\xi)(1+\eta)(1+\zeta)\\
N_{i-1}^{5,8} &= \frac{1}{4}\phi_i(\eta)(1-\xi)(1+\zeta)
\end{aligned}
$$

E.8.3 Face basis

$$
\begin{aligned}
N_{m(i,j)}^{(1,2,5,6)} &= \frac{1}{2}(1-\eta)\phi_i(\xi)\phi_j(\zeta)\\
N_{m(i,j)}^{(1,2,4,3)} &= \frac{1}{2}(1-\zeta)\phi_i(\xi)\phi_j(\eta)\\
N_{m(i,j)}^{(1,4,5,8)} &= \frac{1}{2}(1-\xi)\phi_i(\eta)\phi_j(\zeta)\\
N_{m(i,j)}^{(4,3,8,7)} &= \frac{1}{2}(1+\eta)\phi_i(\xi)\phi_j(\zeta)\\
N_{m(i,j)}^{(5,6,8,7)} &= \frac{1}{2}(1+\zeta)\phi_i(\xi)\phi_j(\eta)\\
N_{m(i,j)}^{(2,3,6,7)} &= \frac{1}{2}(1+\xi)\phi_i(\eta)\phi_j(\zeta)
\end{aligned}
$$

where $i, j = 2, 3, \ldots, p-2$, $i + j = 4, 5, \ldots, p$

E.8.4 Bubble basis

$$
N_{m(i,j,k)}^{(0)} = \phi_i(\xi)\phi_j(\eta)\phi_k(\zeta)
$$

where $i, j, k = 2, 3, \ldots, p-4$, $i + j + k = 6, 7, \ldots, p$

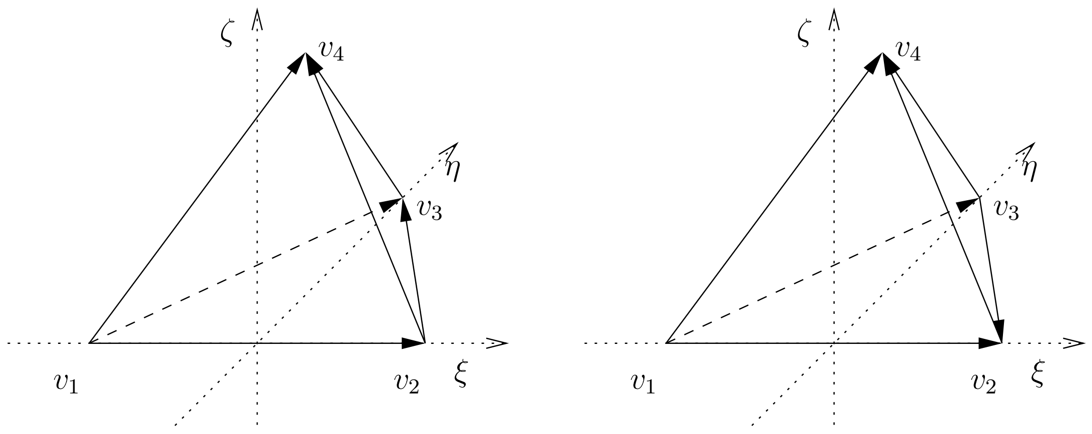


Figure E.7: Tetrahedral elements of types 1 and 2

E.9 Tetrahedron

E.9.1 Nodal basis

$$\begin{aligned}
L_1 &= \frac{1}{2}(1-\xi-\frac{1}{\sqrt{3}}\eta-\frac{1}{\sqrt{6}}\zeta)\\
L_2 &= \frac{1}{2}(1+\xi-\frac{1}{\sqrt{3}}\eta-\frac{1}{\sqrt{6}}\zeta)\\
L_3 &= \frac{\sqrt{3}}{3}(\eta-\frac{1}{\sqrt{8}}\zeta)\\
L_4 &= \sqrt{\frac{3}{8}}\zeta
\end{aligned}$$

E.9.2 Edge basis

Type 1

$$\begin{aligned}
N_{i-1}^{(1,2)} &= L_1L_2\varphi_i(L_2-L_1),\ i=2,\ldots,p\\
N_{i-1}^{(1,3)} &= L_1L_3\varphi_i(L_3-L_1),\ i=2,\ldots,p\\
N_{i-1}^{(1,4)} &= L_1L_4\varphi_i(L_4-L_1),\ i=2,\ldots,p\\
N_{i-1}^{(2,3)} &= L_2L_3\varphi_i(L_3-L_2),\ i=2,\ldots,p\\
N_{i-1}^{(2,4)} &= L_2L_4\varphi_i(L_4-L_2),\ i=2,\ldots,p\\
N_{i-1}^{(3,4)} &= L_3L_4\varphi_i(L_4-L_3),\ i=2,\ldots,p
\end{aligned}$$

Type 2

$$N_{i-1}^{(3,2)} = L_3L_2\varphi_i(L_2-L_3),\ i=2,\ldots,p$$

Edges $(1,2)$,$(1,3)$,$(1,4)$,$(2,4)$ ja $(3,4)$ according to type 1.

E.9.3 Face basis

Type 1

$$
\begin{aligned}
N^{(1,2,3)}_{m(i,j)} &= L_1L_2L_3P_i(L_2-L_1)P_j(2L_3-1)\\
N^{(1,2,4)}_{m(i,j)} &= L_1L_2L_4P_i(L_2-L_1)P_j(2L_4-1)\\
N^{(1,3,4)}_{m(i,j)} &= L_1L_4L_3P_i(L_3-L_1)P_j(2L_4-1)\\
N^{(2,3,4)}_{m(i,j)} &= L_2L_3L_4P_i(L_3-L_2)P_j(2L_4-1)
\end{aligned}
$$

Type 2

$$
\begin{aligned}
N^{(1,3,2)}_{m(i,j)} &= L_1L_3L_2P_i(L_3-L_1)P_j(2L_2-1)\\
N^{(3,2,4)}_{m(i,j)} &= L_3L_2L_4P_i(L_2-L_3)P_j(2L_4-1)
\end{aligned}
$$

where $i,j=0,1,2,\dots,p-3$, $i+j=0,1,\dots,p-3$. Faces $(1,2,4)$ and $(1,3,4)$ defined according to type 1.

E.9.4 Bubble basis

$$N^{(0)}_{m(i,j,k)} = L_1L_2L_3L_4P_i(L_2-L_1)P_j(2L_3-1)P_k(2L_4-1)$$

where $i,j,k=0,1,\dots,p-4$, $i+j+k=0,1,\dots,p-4$

E.10 Pyramid

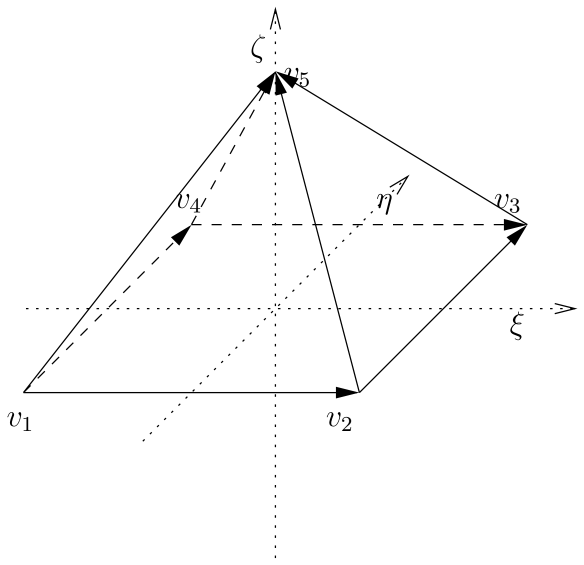


Figure E.8: Pyramidal element

E.10.1 Nodal basis

$$\begin{aligned} T_0(c,t) &= \frac{(1-\frac{t}{\sqrt{2}})-c}{2(1-\frac{t}{\sqrt{2}})} \\ T_1(c,t) &= \frac{(1-\frac{t}{\sqrt{2}})+c}{2(1-\frac{t}{\sqrt{2}})} \end{aligned}$$

$$\begin{aligned} P_1 &= T_0(\xi,\zeta)T_0(\eta,\zeta)(1-\frac{\zeta}{\sqrt{2}}) \\ P_2 &= T_1(\xi,\zeta)T_0(\eta,\zeta)(1-\frac{\zeta}{\sqrt{2}}) \\ P_3 &= T_1(\xi,\zeta)T_1(\eta,\zeta)(1-\frac{\zeta}{\sqrt{2}}) \\ P_4 &= T_0(\xi,\zeta)T_1(\eta,\zeta)(1-\frac{\zeta}{\sqrt{2}}) \\ P_5 &= \frac{1}{\sqrt{2}}\zeta \end{aligned}$$

E.10.2 Edge basis

$$\begin{aligned} P_{i-1}^{(1,2)} &= P_1(\xi,\eta,\zeta)P_2(\xi,\eta,\zeta)\varphi_i(\xi) \\ P_{i-1}^{(2,3)} &= P_2(\xi,\eta,\zeta)P_3(\xi,\eta,\zeta)\varphi_i(\eta) \\ P_{i-1}^{(4,3)} &= P_4(\xi,\eta,\zeta)P_3(\xi,\eta,\zeta)\varphi_i(\xi) \\ P_{i-1}^{(1,4)} &= P_1(\xi,\eta,\zeta)P_4(\xi,\eta,\zeta)\varphi_i(\eta) \\ P_{i-1}^{(1,5)} &= P_1(\xi,\eta,\zeta)P_5(\xi,\eta,\zeta)\varphi_i(\frac{\xi}{2}+\frac{\eta}{2}+\frac{\zeta}{\sqrt{2}}) \\ P_{i-1}^{(2,5)} &= P_2(\xi,\eta,\zeta)P_5(\xi,\eta,\zeta)\varphi_i(-\frac{\xi}{2}+\frac{\eta}{2}+\frac{\zeta}{\sqrt{2}}) \\ P_{i-1}^{(3,5)} &= P_3(\xi,\eta,\zeta)P_5(\xi,\eta,\zeta)\varphi_i(-\frac{\xi}{2}-\frac{\eta}{2}+\frac{\zeta}{\sqrt{2}}) \\ P_{i-1}^{(4,5)} &= P_4(\xi,\eta,\zeta)P_5(\xi,\eta,\zeta)\varphi_i(\frac{\xi}{2}-\frac{\eta}{2}+\frac{\zeta}{\sqrt{2}}) \end{aligned}$$

E.10.3 Face basis

Square face

$$P_{m(i,j)}^{(1,2,3,4)} = P_1(\xi,\eta,\zeta)P_3(\xi,\eta,\zeta)\varphi_i(\xi)\varphi_j(\eta)$$

where $i,j = 2,\dots,p-2$, $i+j = 4,\dots,p$.

Triangular faces

$$\begin{aligned} P_{m(i,j)}^{(1,2,5)} &= P_1(\xi,\eta,\zeta)P_2(\xi,\eta,\zeta)P_5(\xi,\eta,\zeta)P_i(P_2(\xi,\eta,\zeta)-P_1(\xi,\eta,\zeta))P_j(2P_5(\xi,\eta,\zeta)-1) \\ P_{m(i,j)}^{(2,3,5)} &= P_2(\xi,\eta,\zeta)P_3(\xi,\eta,\zeta)P_5(\xi,\eta,\zeta)P_i(P_3(\xi,\eta,\zeta)-P_2(\xi,\eta,\zeta))P_j(2P_5(\xi,\eta,\zeta)-1) \\ P_{m(i,j)}^{(3,4,5)} &= P_3(\xi,\eta,\zeta)P_4(\xi,\eta,\zeta)P_5(\xi,\eta,\zeta)P_i(P_4(\xi,\eta,\zeta)-P_3(\xi,\eta,\zeta))P_j(2P_5(\xi,\eta,\zeta)-1) \\ P_{m(i,j)}^{(4,1,5)} &= P_4(\xi,\eta,\zeta)P_1(\xi,\eta,\zeta)P_5(\xi,\eta,\zeta)P_i(P_1(\xi,\eta,\zeta)-P_4(\xi,\eta,\zeta))P_j(2P_5(\xi,\eta,\zeta)-1) \end{aligned}$$

where $i, j = 0, \ldots, p-3$, $i + j = 0, \ldots, p-3$ and P_i, P_j Legendre polynomials.

E.10.4 Bubble basis

$$P^{(0)}_{m(i,j,k)} = P_1(\xi,\eta,\zeta)P_3(\xi,\eta,\zeta)P_5(\xi,\eta,\zeta)P_i(\frac{\xi}{1-\frac{\zeta}{\sqrt{2}}})P_j(\frac{\eta}{1-\frac{\zeta}{\sqrt{2}}})P_k(\frac{\zeta}{\sqrt{2}})$$

where $i, j, k = 0, \ldots, p-4$, $i + j + k = 0. \ldots, p-4$ and P_i, P_j, P_k Legendre polynomials

E.11 Wedge

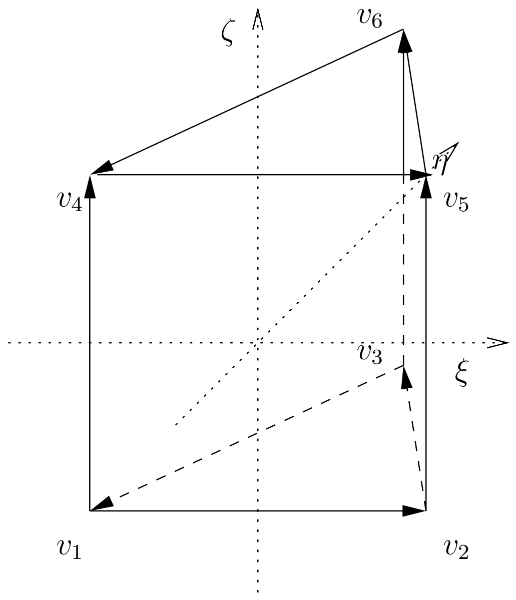


Figure E.9: Wedge element

E.11.1 Nodal basis

$$\begin{aligned} L_1 &= \frac{1}{2}(1 - \xi - \frac{1}{\sqrt{3}}\eta) \\ L_2 &= \frac{1}{2}(1 + \xi - \frac{1}{\sqrt{3}}\eta) \\ L_3 &= \frac{\sqrt{3}}{3}\,\eta \end{aligned}$$

$$
\begin{aligned}
H_1 &= \frac{1}{2}L_1(1-\zeta)\\
H_2 &= \frac{1}{2}L_2(1-\zeta)\\
H_3 &= \frac{1}{2}L_3(1-\zeta)\\
H_4 &= \frac{1}{2}L_1(1+\zeta)\\
H_5 &= \frac{1}{2}L_2(1+\zeta)\\
H_6 &= \frac{1}{2}L_3(1+\zeta)
\end{aligned}
$$

E.11.2 Edge basis

$$
\begin{aligned}
H_{i-1}^{(1,2)} &= \frac{1}{2}L_1L_2\varphi_i(L_2-L_1)(1-\zeta)\\
H_{i-1}^{(2,3)} &= \frac{1}{2}L_2L_3\varphi_i(L_3-L_2)(1-\zeta)\\
H_{i-1}^{(3,1)} &= \frac{1}{2}L_3L_1\varphi_i(L_1-L_3)(1-\zeta)\\
H_{i-1}^{(4,5)} &= \frac{1}{2}L_4L_5\varphi_i(L_5-L_4)(1+\zeta)\\
H_{i-1}^{(5,6)} &= \frac{1}{2}L_5L_6\varphi_i(L_6-L_5)(1+\zeta)\\
H_{i-1}^{(6,4)} &= \frac{1}{2}L_6L_4\varphi_i(L_4-L_6)(1+\zeta)\\
H_{i-1}^{(1,4)} &= L_1\phi_i(\zeta)\\
H_{i-1}^{(2,5)} &= L_2\phi_i(\zeta)\\
H_{i-1}^{(3,6)} &= L_3\phi_i(\zeta)
\end{aligned}
$$

E.11.3 Face basis

Triangular faces

$$
\begin{aligned}
H_{m(i,j)}^{(1,2,3)} &= \frac{1}{2}(1-\zeta)P_i(L_2-L_1)P_j(2L_3-1)L_1L_2L_3\\
H_{m(i,j)}^{(4,5,6)} &= \frac{1}{2}(1+\zeta)P_i(L_2-L_1)P_j(2L_3-1)L_1L_2L_3
\end{aligned}
$$

where $i,j=0,1,\dots,p-3$, $i+j=0,1,\dots,p-3$ and P_i,P_j Legendre polynomials.
Square faces

$$
\begin{aligned}
H_{m(i,j)}^{(1,2,5,4)} &= \varphi_i(L_2-L_1)\phi_j(\zeta)L_1L_2\\
H_{m(i,j)}^{(2,3,6,5)} &= \varphi_i(L_3-L_2)\phi_j(\zeta)L_2L_3\\
H_{m(i,j)}^{(3,1,4,6)} &= \varphi_i(L_1-L_3)\phi_j(\zeta)L_3L_1
\end{aligned}
$$

where $i,j=2,\dots,p-2$, $i+j=4,\dots,p$.

E.11.4 Bubble basis

$$H^{(0)}_{m(i,j,k)} = \phi_k(\zeta)L_1L_2L_3P_i(L_2-L_1)P_j(2L_3-1)$$

where $i, j = 0, \ldots, p-5$, $k = 2, \ldots, p-3$, $i+j+k = 2, \ldots, p-3$.

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