ElmerSolver Command File

Thomas Zwinger

thomas.zwinger[at]csc.fi

Computational Environment & Application
CSC–Scientific Computing Ltd.
The Finnish IT center for science
Espoo, Finland

Contents

The Solver Input File (SIF)

Header

Simulation

Solver

Body

Equation

Bodyforce

Material

Initial Conditions

Boundary Conditions

Bodies on Boundaries

Tables

MATC

User Defined Functions

User Defined Subroutine

Multiple Meshes

Element Types

Specialities

Elmer parallel version

contains all the information for the solution step, ElmerSolver_mpi

- contains all the information for the solution step,
 ElmerSolver_mpi
- can be exported by ElmerGUI (also ElmerFront) ...

- contains all the information for the solution step, ElmerSolver_mpi
- can be exported by ElmerGUI (also ElmerFront)
- ... but simply also composed using a text editor

- contains all the information for the solution step, ElmerSolver_mpi
- can be exported by ElmerGUI (also ElmerFront)...
- ... but simply also composed using a text editor

- contains all the information for the solution step, ElmerSolver_mpi
- can be exported by ElmerGUI (also ElmerFront) ...
- ... but simply also composed using a text editor

The Rules:

comments start with !

- contains all the information for the solution step, ElmerSolver_mpi
- can be exported by ElmerGUI (also ElmerFront)
- ... but simply also composed using a text editor

- comments start with !
- Important: do not use tabulators for indents!

- contains all the information for the solution step, ElmerSolver_mpi
- can be exported by ElmerGUI (also ElmerFront)
- ... but simply also composed using a text editor

- comments start with !
- Important: do not use tabulators for indents!
- a section always ends with the keyword End

- contains all the information for the solution step, ElmerSolver_mpi
- can be exported by ElmerGUI (also ElmerFront)
- ... but simply also composed using a text editor

- comments start with !
- Important: do not use tabulators for indents!
- a section always ends with the keyword End
- parameters (except from Elmer keyword database) need to be casted by their types: Integer Real Logical String File

- contains all the information for the solution step, ElmerSolver_mpi
- can be exported by ElmerGUI (also ElmerFront)
- ... but simply also composed using a text editor

- comments start with !
- Important: do not use tabulators for indents!
- a section always ends with the keyword End
- parameters (except from Elmer keyword database) need to be casted by their types: Integer Real Logical String File
- Parametername(n,m) indicates a $n \times m$ array

Header

The header declares where to search for the mesh database

```
Header
    Mesh DB "." "dirname"
End
```

preceding path + directory name of mesh database

Constants

Declaration of constant values that can be obtained from within **every** solver and boundary condition **subroutine** or **function**, can be declared.

```
Constants

Gas Constant = Real 8.314E00

Gravity (4) = 0 -1 0 9.81

End
```

a scalar constant

Gravity vector, an array with a registered name

Simulation

Principle declarations for simulation

```
Simulation
  Coordinate System = "Cartesian 2D"
  Coordinate Mapping(3) = Integer 1 2 3
  Simulation Type = "Steady"
  Output Intervals = 1
  Steady State Max Iterations = 10
  Steady State Min Iterations = 2
  Output File = "name.result"
  Post File = "name.ep"
  \max \text{ output level } = n
```

choices: Cartesian {1D,2D,3D}, Polar {2D,3D}, Cylindric, Cylindric Symmetric, Axi Symmetric permute, if you want to interchange directions either Steady or Transient how often you want to have results maximum rounds on one time level minimum rounds on one Timestep contains data to restart run ElmerPost-file n=1 talkative like a Finnish lumberjack, n=42 all and everything

End

Solver

Example: (Navier) Stokes solver

```
Solver 1
  Equation = "Navier-Stokes"
  Linear System Solver = "Direct"
  Linear System Direct Method = "UMFPack"
  Linear System Convergence Tolerance = 1.0E-06
  Linear System Abort Not Converged = True
  Steady State Convergence Tolerance = 1.0E-03
  Stabilization Method = Stabilized
  Nonlinear System Convergence Tolerance = 1.0E-05
  Nonlinear System Max Iterations = 40
  Nonlinear System Min Iterations = 1
  Nonlinear System Newton After Iterations = 30
  Nonlinear System Newton After Tolerance = 1.0E-05
End
```

name of the solver alt. Iterative

not used

a non-linear problem

Newton iter.

Body

Here the different bodies (there can be more than one) get their Equation, Material, Body Force and Initial Condition assigned

```
Body 2
Name = "identifier"
Equation = 1
Material = 2
Body Force = 1
Initial Condition = 1
End
```

```
there can be more than one body
give the body a name
one Equation/Material/
Body Force/Initial Condition
can serve several bodies
```

Equation

- set active solvers
- give keywords for the behaviour of different solvers

```
Equation 1
  Active Solvers(2) = 1 2
  Convection = Computed
  Flow Solution Name = String "Flow Solution"
  NS Convect = False
End
```

Bodyforce

- lacktriangledown declares the solver-specific f from $A\cdot\Psi=f$ for the body
- body force can also be a dependent function (see later).

Here for the (Navier) Stokes solver

```
Body Force 1

Flow BodyForce 1 = 0.0

Flow BodyForce 2 = -9.81 ! good old gravity

End
```

Material

- sets material properties for the body.
- material properties can be scalars or tensors and also
- can be given as dependent function/expression

```
Material 1
  Density = 918.0
  Heat Capacity = Variable Temperature
  MATC "2.1275D03 + 7.253D00*(tx - 273.16)"
  My Variable = Real 1002.0
End
```

dependence
a MATC expression (see later)
not in keyword DB!

Initial Conditions

- initializes variable values
- sets initial guess for steady state simulation
- sets initial value for transient simulation
- variable values can be functions/expressions

Boundary Conditions

- Dirichlet: variablename = value
- Neumann: often enabled with keyword (e.g., HTEqu. Heat Flux
 BC = True) followed by the flux value
- No BC

 Natural BC!
- values can be given as functions

Example: (Navier) Stokes with no penetration (normal) and free slip (tangential)

```
Boundary Condition 1
Name = "slip"
Target Boundaries = 4
Normal-Tangential Velocity = Logical True
Velocity 1 = Real 0.0
End
```

name
refers to boundary no. 4 in mesh
components with respect to surface normal
normal component

 need to solve (dimension-1) PDEs (e.g., kinematic BC on free surface)

- need to solve (dimension-1) PDEs (e.g., kinematic BC on free surface)
- need to define the (dimension-1) entity as a separate body

- need to solve (dimension-1) PDEs (e.g., kinematic BC on free surface)
- need to define the (dimension-1) entity as a separate body
- in the corresponding Boundary-section:

Body ID = n with n > highest occurring body in the mesh

- need to solve (dimension-1) PDEs (e.g., kinematic BC on free surface)
- need to define the (dimension-1) entity as a separate body
- define Body Force, Material, Equation and Initial Condition for that body

- need to solve (dimension-1) PDEs (e.g., kinematic BC on free surface)
- need to define the (dimension-1) entity as a separate body
- define Body Force, Material, Equation and Initial Condition for that body
- full dimensional metric is still valid on the BC body \Rightarrow has to be taken into account in user supplied subroutines

Tables may be used for piecewise linear dependency of a variable

Tables may be used for piecewise linear dependency of a variable

```
Density = Variable Temperature

Real

0 900

273 1000

300 1020

400 1000

End
```

Tables may be used for piecewise linear dependency of a variable

```
Density = Variable Temperature

Real

0 900
273 1000
300 1020
400 1000
End
```

Arrays may be used to declare vector/tensor parameters

Tables may be used for piecewise linear dependency of a variable

```
Density = Variable Temperature

Real

0 900

273 1000

300 1020

400 1000

End
```

Arrays may be used to declare vector/tensor parameters

library for the numerical evaluation of mathematical expressions

- library for the numerical evaluation of mathematical expressions
- defined in SIF for use in ElmerSolver

- library for the numerical evaluation of mathematical expressions
- defined in SIF for use in ElmerSolver
- or by ElmerPost as post-processing feature

e.g.
$$K \rightarrow {}^{\circ}C$$
: math Celsius = Temperature + 273.16

- library for the numerical evaluation of mathematical expressions
- defined in SIF for use in ElmerSolver
- or by ElmerPost as post-processing feature e.g. $K \rightarrow {}^{\circ}C$: math Celsius = Temperature + 273.16
- very close to C-syntax

- library for the numerical evaluation of mathematical expressions
- defined in SIF for use in ElmerSolver
- or by ElmerPost as post-processing feature e.g. $K \rightarrow {}^{\circ}C$: math Celsius = Temperature + 273.16
- very close to C-syntaxalso logical evaluations (if) and loops (for)

- library for the numerical evaluation of mathematical expressions
- defined in SIF for use in ElmerSolver
- or by ElmerPost as post-processing feature e.g. $K \rightarrow {}^{\circ}C$: math Celsius = Temperature + 273.16
- very close to C-syntaxalso logical evaluations (if) and loops (for)
- documentation on Funet (MATC Manual)

simple numerical evaluation:

```
Viscosity Exponent = Real MATC "1.0/3.0" Of
Viscosity Exponent = Real $1.0/3.0
```

simple numerical evaluation:

```
Viscosity Exponent = Real MATC "1.0/3.0" Or
Viscosity Exponent = Real $1.0/3.0
```

as an expression dependent on a variable:

```
Heat Capacity = Variable Temperature
Real MATC "2.1275D03 + 7.253D00*(tx - 273.16)"
```

simple numerical evaluation:

```
Viscosity Exponent = Real MATC "1.0/3.0" Or
Viscosity Exponent = Real $1.0/3.0
```

as an expression dependent on a variable:

```
Heat Capacity = Variable Temperature
Real MATC "2.1275D03 + 7.253D00*(tx - 273.16)"
```

as an expression of multiple variables:

```
Temp = Variable Latitude, Coordinate 3
Real MATC "49.13 + 273.16 - 0.7576 * tx(0) - 7.992E-03 * tx(1)"
```

simple numerical evaluation:

```
Viscosity Exponent = Real MATC "1.0/3.0" Or
Viscosity Exponent = Real $1.0/3.0
```

as an expression dependent on a variable:

```
Heat Capacity = Variable Temperature
Real MATC "2.1275D03 + 7.253D00*(tx - 273.16)"
```

as an expression of multiple variables:

```
Temp = Variable Latitude, Coordinate 3
Real MATC "49.13 + 273.16 - 0.7576 * tx(0) - 7.992E-03 * tx(1)"
```

as function defined at the top of SIF:

```
Temp = Variable Latitude, Coordinate 3
Real MATC "stemp(tx)"
```

Example: $\rho(T(^{\circ}C)) = 1000 \cdot [1 - 10^{-4} \cdot (T - 273.0)]$

Example: $\rho(T(^{\circ}C)) = 1000 \cdot [1 - 10^{-4} \cdot (T - 273.0)]$

```
FUNCTION getdensity( 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 getdensity
```

Example: $\rho(T(^{\circ}C)) = 1000 \cdot [1 - 10^{-4} \cdot (T - 273.0)]$

```
FUNCTION getdensity( 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 getdensity
```

compile: elmerf90 mydensity.f90 -o mydensity

Example: $\rho(T(^{\circ}C)) = 1000 \cdot [1 - 10^{-4} \cdot (T - 273.0)]$

```
FUNCTION getdensity( 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 getdensity
```

compile: elmerf90 mydensity.f90 -o mydensity

```
RECURSIVE SUBROUTINE &

mysolver( Model,Solver,dt,TransientSimulation )

TYPE(Model_t) :: Model

TYPE(Solver_t) :: Solver

REAL(KIND=dp) :: dt

LOGICAL :: TransientSimulation
...

assembly, solution
...

END SUBROUTINE mysolver
```

```
RECURSIVE SUBROUTINE &
mysolver( Model, Solver, dt, TransientSimulation )
TYPE(Model_t) :: Model
TYPE(Solver_t) :: Solver
REAL(KIND=dp) :: dt
LOGICAL :: TransientSimulation
assembly, solution
END SUBROUTINE mysolver
```

```
Model pointer to the whole Model (solvers, variables)

Solver pointer to the particular solver

dt current time step size

TransientSimulation .TRUE. if transient simulation
```

```
RECURSIVE SUBROUTINE &
mysolver( Model, Solver, dt, TransientSimulation )
TYPE(Model_t) :: Model
TYPE(Solver_t) :: Solver
REAL(KIND=dp) :: dt
LOGICAL :: TransientSimulation
...
assembly, solution
...
END SUBROUTINE mysolver
```

```
Model pointer to the whole Model (solvers, variables)

Solver pointer to the particular solver

dt current time step size

TransientSimulation .TRUE. if transient simulation

elmerf90 mysolverfile.f90 -o mysolverexe
```

compile:



```
RECURSIVE SUBROUTINE &
mysolver( Model, Solver, dt, TransientSimulation )
TYPE(Model_t) :: Model
TYPE(Solver_t) :: Solver
REAL(KIND=dp) :: dt
LOGICAL :: TransientSimulation
assembly, solution
END SUBROUTINE mysolver
                Model
                        pointer to the whole Model (solvers, variables)
```

```
Model pointer to the whole Model (solvers, variables)

Solver pointer to the particular solver

dt current time step size

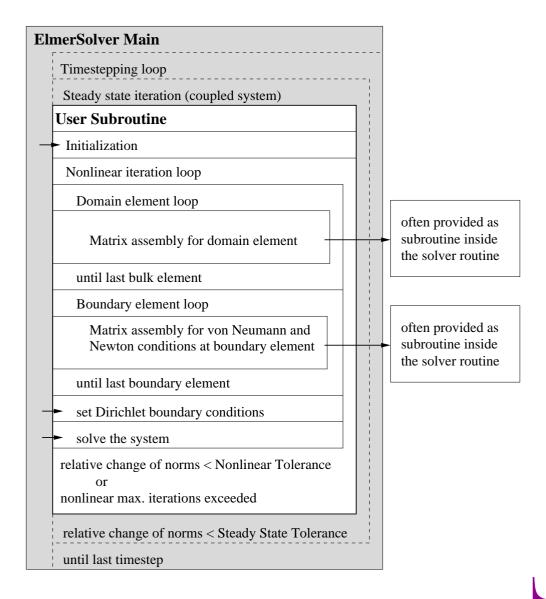
TransientSimulation .TRUE. if transient simulation

compile: elmerf90 mysolverfile.f90 -o mysolverexe
```

SIF:

Procedure = "/path/to/mysolverexe" "mysolver"

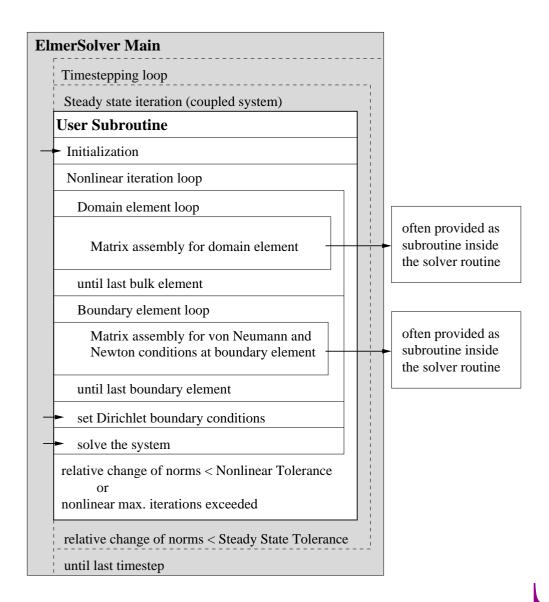
User Defi ned Subroutines contd.



User Defi ned Subroutines contd.

Pre-defined routines

- CALL
 DefaultInitialize()
- DefaultUpdateEquations(
 STIFF, FORCE)
- CALL
 DefaultFinishAssembly()
- CALL
 DefaultDirichletBCs()
- Norm =
 DefaultSolve()



In the Header, declare the *global* mesh database

```
Mesh DB "." "dirname"
```

In the Header, declare the *global* mesh database

```
Mesh DB "." "dirname"
```

In the Solver, declare the local mesh the solver is run on:

```
Mesh = File "/path/to/" "mesh"
```

In the Header, declare the *global* mesh database

```
Mesh DB "." "dirname"
```

In the Solver, declare the local mesh the solver is run on:

```
Mesh = File "/path/to/" "mesh"
```

variable values will be interpolated

In the Header, declare the *global* mesh database

```
Mesh DB "." "dirname"
```

In the Solver, declare the local mesh the solver is run on:

```
Mesh = File "/path/to/" "mesh"
```

variable values will be interpolated

they will boldly be extrapolated, should your meshes not be congruent!

● In section Equation:

In section Equation:

```
Element = [n:#dofs d:#dofs p:#dofs b:#dofs e:#dofs f:#dofs]
n...nodal, d...DG element, pp-element, b...bubble, e...edge, f...face DOFs
```

● In section Equation:

```
Element = [n:#dofs d:#dofs p:#dofs b:#dofs e:#dofs f:#dofs]
n...nodal, d...DG element, pp-element, b...bubble, e...edge, f...face DOFs
```

lacktriangle Element = [d:0] ... DG DOFs \equiv mesh element nodes

● In section Equation:

```
Element = [n:#dofs d:#dofs p:#dofs b:#dofs e:#dofs f:#dofs]
n...nodal, d...DG element, p.p-element, b...bubble, e...edge, f...face DOFs
```

- Element = [d:0] ... DG DOFs \equiv mesh element nodes
- If Equation applies to more than one solver, Element = ... applies for all solver.

● In section Equation:

```
Element = [n:#dofs d:#dofs p:#dofs b:#dofs e:#dofs f:#dofs]
n...nodal, d...DG element, p.p-element, b...bubble, e...edge, f...face DOFs
```

- Element = [d:0] ... DG DOFs \equiv mesh element nodes
- If Equation applies to more than one solver, Element = ... applies for all solver.

selectively for each solver: Element[1] = ...

```
Element[2] = ...

:
:
:
:
Element[n] = ...
```

given names for components of vector fields:

```
Variable = var_name[cname 1:#dofs cname 2:#dofs ... ]
```

given names for components of vector fields:

```
Variable = var_name[cname 1:#dofs cname 2:#dofs ... ]
```

 "internal" Solver can be run as external Procedure (enabling definition of variable names)

```
Procedure = "FlowSolve" "FlowSolver"

Variable = Flow[Veloc:3 Pres:1]
```

given names for components of vector fields:

```
Variable = var_name[cname 1:#dofs cname 2:#dofs ... ]
```

 "internal" Solver can be run as external Procedure (enabling definition of variable names)

```
Procedure = "FlowSolve" "FlowSolver"

Variable = Flow[Veloc:3 Pres:1]
```

Residuals of solver variables (e.g., Navier Stokes):

```
Procedure = "FlowSolve" "FlowSolver"

Variable = Flow[Veloc:3 Pres:1]

Exported Variable 1 = Flow Loads[Stress Vector:3 CEQ Residual:1]
```

given names for components of vector fields:

```
Variable = var_name[cname 1:#dofs cname 2:#dofs ... ]
```

 "internal" Solver can be run as external Procedure (enabling definition of variable names)

```
Procedure = "FlowSolve" "FlowSolver"

Variable = Flow[Veloc:3 Pres:1]
```

Residuals of solver variables (e.g., Navier Stokes):

```
Procedure = "FlowSolve" "FlowSolver"

Variable = Flow[Veloc:3 Pres:1]

Exported Variable 1 = Flow Loads[Stress Vector:3 CEQ Residual:1]
```

Solver execution:

```
Exec Solver = {Before Simulation, After Simulation, Never, Always}
```

Elmer Parallel Version

Pre-processing: ElmerGrid with options:

Partition by direction:

```
-partition 2 2 1 0 First partition elements (default)

-partition 2 2 1 1 First partition nodes 2 \times 2 \times = 4
```

Partition using METIS:

```
-metis n 0 PartMeshNodal (default)

-metis n 1 PartGraphRecursive

-metis n 2 PartGraphKway

-metis n 3 PartGraphVKway
```

Elmer Parallel Version

Pre-processing: ElmerGrid with options:

Partition by direction:

```
-partition 2 2 1 0 First partition elements (default) -partition 2 2 1 1 First partition nodes 2 \times 2 \times = 4
```

Partition using METIS:

```
-metis n 0 PartMeshNodal (default)
-metis n 1 PartGraphRecursive
-metis n 2 PartGraphKway
-metis n 3 PartGraphVKway
```

Execution: mpirun -np n ElmerSolver_mpi

Elmer Parallel Version

Pre-processing: ElmerGrid with options:

Partition by direction:

```
-partition 2 2 1 0 First partition elements (default)

-partition 2 2 1 1 First partition nodes 2 \times 2 \times = 4
```

Partition using METIS:

```
-metis n 0 PartMeshNodal (default)
-metis n 1 PartGraphRecursive
-metis n 2 PartGraphKway
-metis n 3 PartGraphVKway
```

- Execution: mpirun -np n ElmerSolver_mpi
- Combining parallel results: in mesh-database directory

```
ElmerGrid 15 3 name
```