Elmer FEM Webinar Series

CSC, Espoo, Finland via Zoom Thursdays 15 EET, 14 CET, 8 ET, 22 JST Spring 2021

Practical guidelines for the webinar



- Chat may be used for general discussion • You may write about your application area, geographic location etc.
- The presentation slides will be made available at <u>https://www.nic.funet.fi/pub/sci/physics/elmer/webinar/</u>
- This webinar will be recorded and will for most parts be available later on youtube



Elmer FEM webinar series - program

- 11.3. Peter Råback & Thomas Zwinger: *Introduction to Elmer & How to teach yourself Elmer*
- 18.3. Peter Råback & Jonathan Velasco: Overview of capabilities of Elmer where to go from here?
- 25.3. Peter Råback & Thomas Zwinger: *Parallel Computing with Elmer*
- 1.4. Juris Vencels: *Elmer-OpenFOAM library*
- 8.4. Eelis Takala & Frederic Trillaud: *Electrical circuits with Elmer with applications*
- 15.4. Mika Malinen: Solvers for solid mechanics Recent progress
- 22.4. Minhaj Zaheer: Induction Machine Open-source FEA Computations comparison with Measurement and Commercial FEA
- 29.4. Arved Enders-Seidlitz: *pyelmer Python interface for Elmer workflow*
- 13.5. Roman Szewczyk, Anna Ostaszewska-Liżewska, Dominika Kopala & Jakub Szałatkiewicz: Industrial applications oriented, microwave modelling in Elmer
- Additional slots available: contact organizers if you're interested!

Overview of capabilities of Elmer

ElmerTeam CSC – IT Center for Science, Finland

Elmer FEM webinar

2021

Outline for today

- Overview of physical models
 - o From Models Manual
 - Example: 12 Solvers
- Library features used by many/all models

 Iteration scheme & coupling
 Generality of fetching Real valued keywords
 Executions of solver
 - Time dependency modes
 - Bounday conditions
 - Mapping between boundaries and meshes
 - 0...
- Where to go next?

Example of minimal sif file

! Minimal sif file example Check Keywords "Warn"

```
Header :: Mesh DB "." "square"
```

Simulation

```
Max Output Level = 5
Coordinate System = Cartesian
Simulation Type = Steady
Output Intervals(1) = 1
Steady State Max Iterations = 1
Post File = "case.vtu"
End
```

Body 1 Equation = 1 Material = 1

```
End
```

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

Solver 1



Elmer – abstraction of Solvers

- High level of abstraction ensures flexibility in implementation and simulation
- Solver is an asbtract dynamically loaded object with standard API

 Solver may be developed and compiled without touching the main library
 No upper limit to the number of Solvers
- Solvers may be active in different domains, and even meshes • Automatic mapping of field values when requested!
- Solvers perform limited well defined tasks
 - \odot Solution of a PDE (roughly 50%)
 - \circ Computing some postprocessed fields
 - Saving of results

0

• Solver may utilize a large selection of services from the library • The library has (almost) no knowledge of physical models

Physical Models of Elmer -> Elmer Models Manual

• Heat transfer

- \checkmark Heat equation
- \checkmark Radiation with view factors
- \checkmark convection and phase change
- Fluid mechanics
 - ✓ Navier-Stokes (2D & 3D)
 - ✓ RANS: SST k- Ω , k- ε , v²-f
 - ✓ LES: VMS
 - ✓ Thin films: Reynolds (1D & 2D)
- Structural mechanics
 - ✓ General elasticity (unisotropic, lin & nonlin)
 - ✓ Plates & Shells
- Acoustics
 - ✓ Helmholtz
 - ✓ Linearized time-harmonic N-S
 - ✓ Monolithic thermal N-S
- Species transport
 - ✓ Generic convection-diffusion equation

- Electromagnetics
 - Solvers for either scalar or vector potential (nodal elements)

- Edge element based AV solver for magnetic and electric fields
- Mesh movement (Lagrangian)
 - Extending displacements in free surface problems
 - ✓ ALE formulation
- Level set method (Eulerian)
 - \checkmark Free surface defined by a function
- Electrokinetics
 - ✓ Poisson-Boltzmann
- Thermoelectricity
- Quantum mechanics
 ✓ DFT (Kohn Scham)
- Particle Tracker

Most important physical modules in Elmer?

Historically main solver in each field

HeatSolve

Heat equation
Radiation with view factors
convection and phase change

• FlowSolve

Robust solver for low Re-flows
Nonlinear fluids, slip conditions,...
Key solver for Elmer/Ice community

• StressSolve

Versatile solver for linear elasticity

WhitneyAVSolver

18.3.2021

o Hcurl conforming elementso Key solver for Elmer/EM community

Solvers with unresolved potential

ShellSolver

 Enables economical treatment of thin structures

 $_{\odot}$ Now can be combined with 3D elasticity

VectorHelmholtz

Hcurl basis
 Electromagnetics wave solver

ModelMixedPoisson

Hybrid solution employing Hdiv basis

ParticleAdvector

- Uses particles to advect fields without diffusion
- Particles & finite elements often a good combination





Series 1. Question 1. (one choice)

• Number of solvers in your most complicated Elmer simulation setup so far?

CSC

 \circ Zero

 $\mathbf{O}\mathbf{1}$

02-3

04-6

07-10

 \odot >10

Undocumented Models

AllocateSolver.F90	% just dummy solver for allocation	OdeSolver.F90	% ordinary differential equation solver
CoordinateTransform.F90 % RotMSolver: using distances create direction			% partition mesh solver
• •	0 % model reduction solver	PoissonDG.F90	
DCRComplexSolve.F90	% complex diffusion-convection-reaction	Poisson.F90	
DFTSolver.F90	% charge density using the eigenvectors	• •	90 % reduction of rigid pieces
DirectionSolver.F90		SaveMesh.F90	% mesh saving
DistanceSolve.F90	% compute distance in two methods	ScannedFieldSolver.F9	0 % treating scanned field solutions
DistributeSource.F90	% local to global mesh sources	ShallowWaterNS.F90	
ElementSizeSolver.F90	% element size with Galerkin	ShearrateSolver.F90	
EliminateDirichlet.F90		Spalart-Allmaras.F90	% turbulence
EliminatePeriodic.F90		SSTKomega.F90	% turbulence
EnergyRelease.F90	% energy release rate for crack propagation	StatCurrentSolveVec.F	90 % new version of StatCurrentSolve
FacetShellSolve.F90		ThermoElectricSolver.F90 % strongly coupled thermal & electrostatics	
FDiffusion3D.F90	% Complex nodal equation for vector fields	TransientCost.F90	% integral over cost
FDiffusion.F90	% Complex nodal equation for scalar fields	UMATLib.F90	
HeatSolveVec.F90	% new generation HeatSolve	V2FSolver.F90	% turbulence
HelmholtzProjection.F9	0 % purifying vector potential	WPotentialSolver.F90	% potential for directions
IncompressibleNSVec.F	90 % new generation flowsolve		
KESolver.F90	% turbulence	• 76 models have	been documented
Komega.F90	% turbulence	 Tens of modules have not been documented! Some are of little use but might find users if people would find them. 5 undocumented turbulence models exist but they 	
Mesh2MeshSolver.F90	% interpolation		
MeshChecksum.F90	% utility to check mesh consistency		
ModelPDE.F90	% simple advection-diffusion-reaction		
	% calculate normal		
		are not that rob	oust

Example: TwelveSolvers2D

- The purpose of the example is to show how number of different solvers are used
- The users should not be afraid to add new atomistic solvers to perform specific tasks
- A case of 12 solvers is rather rare, yet not totally unrealitistic
- Added now also as test case

- Square with hot and cold walls
- Filled with viscous fluid
- Bouyancy modeled with Boussinesq approximation
- Temperature difference initiates a convection roll



test case: TwelveSolvers2D



Example: the 12 solvers

1. HeatSolver





- 3. FluxSolver: solve the heat flux
- 4. StreamSolver: solve the stream function
- 5. VorticitySolver: solve the vorticity field (curl of vector field)
- 6. DivergenceSolver: solve the divergence
- 7. ShearrateSolver: calculate the shearrate
- 8. IsosurfaceSolver: generate an isosurface at given value
- 9. ResultOutputSolver: write data
- 10. SaveGridData: save data on uniform grid
- **11.** SaveLine: save data on given lines
- **12.** SaveScalars: save various reductions



Mesh of 10000 bilinear elements

Example: Primary fields for natural convection





CSC

Pressure

Temperature



Example: Derived fields for Navier-Stokes solution





Example: Derived fields for heat equation





 Nodal loads only occur at boundaries (nonzero heat source)

 Nodal loads are associated to continuous heat flux by element size factor

Heat flux

Nodal heat loads

Example: Visualization in different postprocessors



GiD

Paraview

Example: total flux

- Saved by SaveScalars
- Two ways of computing the total flux give different approximations
- When convergence is reached the agreement is good



Example: boundary flux

- Saved by SaveLine
- Three ways of computing the boundary flux give different approximations
- At the corner the nodal flux should be normalized using only *h*/*2*



Some common features for PDE solvers

- Iteration scheme & coupling: linear, nonlinear & steady state level
- Generalized fetching of keywords
- Execution of Solvers
- Time dependency modes
- Finite element basis
- Dirichlet BCs
- Nodal loads

• ...

24

- Shared boundary conditions
- Overlapping meshes

18.3.2021

Nested iterations in Elmer as defined by the SIF file



Solution of linear system

- Keywords starting with "Linear System"
- The lowest level operation
- Tens of different techqniques in serial and parallel
- We will go through these next week!

Solution of nonlinear system



The level for iterating over one single nonlinear equation
 By default ElmerGUI assumes nonlinear iteration => always two iterations

Solver i

Nonlinear System Max Iterations = Integer Nonlinear System Convergence Tolerance = Real Nonlinear System Relaxation Factor = Real Nonlinear System Convergence Measure = String Nonlinear System Newton After Tolerance = Real Nonlinear System Newton After Iterations = Real Nonlinear system consistent norm = Logical

$$u_{i}^{\prime} = \lambda u_{i} + (1 - \lambda)u_{i-1}$$

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

"solution"

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

"residual"

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

...

Solution of coupled system



- Keywords starting with "Steady State"
- The level for iterating over set of Solvers to find the solution satisfying all of them

Simulation Steady State Max Iterations = Integer Steady State Min Iterations = Integer

Solver i Steady State Convergence Tolerance = Real Steady State Relaxation Factor = Real Steady State Convergence Measure = Real

28 18.3.2021

...

Solution strategies for coupled problems



Assume phenomena \mathcal{F} and \mathcal{G} that both depend on field variables x and y. Solution is obtained from a system of equations, f(x, y) = 0 and g(y, x) = 0.

one-directional coupling \Rightarrow hierarchical solution

 $\begin{array}{rcl} f(x_1) &= 0 \\ \Rightarrow & g(y_1, x_1) &= 0 \end{array}$

CSC

weak coupling \Rightarrow iterative or segregated solution

 $\begin{cases} f(x_{m+1}, y_m) &= 0\\ g(y_{m+1}, x_{m+1}) &= 0 \end{cases}$

strong coupling \Rightarrow monolithic solution

 $\begin{bmatrix} f(x_{m+1}, y_{m+1})\\ g(y_{m+1}, x_{m+1}) \end{bmatrix} = \begin{bmatrix} 0\\ 0 \end{bmatrix}$

Monolithic approach requires iteration if either f or g is nonlinear.

Weak coupling in Elmer

- Parameters in equations depend on field values

 Nonlinear iteration within on Solver
 Coupled system iteration among solvers
- Consistency in ensured within nested iterations
- E.g. case of natural convection
 - Force on the Navier-Stokes depends on the temperature of the heat equation
 - Convection velocity in the heat equation depends on the solution of the Navier-Stokes equation
- Some dependencies have been "coded in" while others take use of the generic way to give **Real** valued keywords in Elmer

Real valued keyword functions

1) Tables can be use to define a piecewise linear (or cubic) dependency of a variable Density = Variable Temperature Real cubic 173 990 273 1000 373 1010 End Outside range: Extrapolation!

2) MATC: a library for numerical evaluation of mathematical expressions Density = Variable Temperature MATC "1000*(1 - 1.0e-4*(tx(0)-273.0))" or as constant expressions

```
3) LUA: external library, faster than MATC
Density = Variable Temperature
LUA "1000*(1 - 1.0e-4*(tx[0]-273.0))"
```

```
4) User defined function
Density = Variable Temperature
Procedure "mymodule" "myproc"
```

Four ways to present: $\rho = \rho_0(1 - \alpha(T - T_0)))$



Example of F90 User Function

CSC

File mymodule.F90:

```
FUNCTION myproc( 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-273.0_dp))
END FUNCTION myproc
```

Compilation script comes with installation: **elmerf90**

Linux

```
$ elmerf90 mymodule.F90 -o mymodule.so
Windows
$ elmerf90 mymodule.F90 -o mymodule.dll
```

ElmerSolver - Controlling execution order of Solvers

- By default each a Solver is executed in order of their numbering numbering
- "Exec Solver" keyword can be used to alter this
 - o "always" execute in the coupled system loop of the nested iteration
 - \circ "before all" or "before simulation" -
 - o "after all" or "after simulation" perform something
 - o "before saving" perform before saving sequence, maybe compute something for saving
 - o "after saving" perform after saving sequence, maybe save someting
 - o"before timestep" perform before timestep only
 - o "after timestep" perform after timestep only
 - o"never" skip solver for debugging etc.
- "Slave solver" slots (rather new feature) may be used to have some master Solver call other solvers within their execution.

 \circ Added flexibility to complex cases

ElmerSolver – Time dependency modes

• Transient simulation

o ist order PDEs:

Backward differences formulae (BDF) up to 6th degree
 Newmark Beta (Cranck-Nicolsen with β=0.5)
 2nd order Runge-Kutta
 Adaptive timestepping
 2nd order PDEs:
 Bossak

- Steady-state simulation
- Scanning

 $\odot\,\mbox{Special}$ mode for parametric studies etc.

- Harmonic simulation
- Eigenmode simulation
 - $_{\odot}$ Utilizes (P)Arpack library

Simulation Simulation Type = Transient Timestep Intervals = 100 Timestep Sizes = 0.1 Timestepping Method = implicit euler

Simulation Type = Steady

Simulation Type = Scanning



Eigen Analysis

- Any 2nd order PDE may be solved as an eigen system
 od/dt -> iω
- Example, eigenmodes from Smitc, the plate equation

Solver i

Eigen Analysis = True Eigen System Values = 10 Eigen System Convergence Tolerance = 1.0e-6 Eigen System Select = Smallest Magnitude



ElmerSolver – Finite element shapes

- Element shapes are define already in the mesh files Ð
- oD: vertex Ð
- 1D: edge Ð
- 2D: triangles, quadrilateral Ð
- 3D: tetrahedrons, prisms, pyramids, hexahedrons



base

Hexahedron



ElmerSolver – Finite element basis functions

- Element types and formulations are applied on elements
 Solver-wise
- Element families
 - Nodal (up to 2-4th degree)
 - p-elements (hierarchical basis)
 - Edge & face –elements
 - H(div) often associated with "face" elements)
 - H(curl) often associated with "edge" elements)
- Formulations
 - Galerkin, Discontinuous Galerkin
 - Stabilization
 - Residual free bubbles







Examples of FEM basis

- Different equations may require different basis functions beyond the standard nodal finite element basis
- Solvers supporting p-elements (here 3rd order), e.g. ModelPDE
 Element = p:3
- Lowest order *Hcurl* elements for WhitneyAVSolver
 Element = n:1 e:1 ! Hidden from end-user
- Lowest order *Hdiv* elements for ModelMixedPoisson
 Element = n:o -tetra b:1 -brick b:25 -quad_face b:4 -tri_face b:1 ! Hidded from end-user

•

ElmerSolver: Exported Variables

- Any solver may allocate additional variables called "Exported Variables"
- These may be used for various uses, for example create derived fields easily
 - May be used in the same way for "Initial Condition" as regular variables.
 - May be updated if defined in "Body Force" section and "Update Exported Variables" is requested.
- Often defined inside the code
- Exported variables may be of different types o-nodal, -elem, -dg, -ip

A – Arrhenius constant (frequency factor) E_{σ} – activation energy (J mol⁻¹) R – gas constant (8.31 J K⁻¹ mol⁻¹)

#R=8.31 #Ea=123.4 #A=5.67e-3

Solver i Exported Variable 1 = Rate Updated Exported Variables = True

Body Force j Rate = Variable "Tempeture" Real LUA "A0*exp(-Eact/(R*tx[0]))"

ElmerSolver - Dirichlet Conditions

• Dirichlet keywords are set by the library for "Varname"

o Temperature = 273.0

O Velocity = Variable "Coordinate 2"; Real LUA "4*tx[0]*(1-tx[0])"

- AV {e} = o.o ! For edge degree of freedom
- Conditional Dirichelt conditions "Varname Condition"
 Applied only when condition is positive
 - Temperature = 273.0
 Temperature Condition = Equals "Velocity 1" ! Set temperature for inflow only
- Boundary Condition i
- Body Force i

 \odot Enables bodywise Dirichlet conditions also
ElmerSolver – Computing nodal forces

- ElmerSolver allows for automatic computation of nodal forces from matrix equation: f=A_ox-b
- These are reactions to Dirichlet conditions that give equivalent r.h.s. terms that would result in exactly the same solution
 - O HeatSolver: nodal heat flux (Joule)
 - o FlowSolve: nodal force (Newton)
 - o StressSolve: nodal force (Newton)
 - o StatElecSolve: nodal charge (Coulomb)
 - o StatCurrentSolve: nodal current (Ampere)
- Coupling between two solvers may be done either on the continuous or discrete level

Solver i Calculate Loads = True

ElmerSolver – Setting nodal forces

- ElmerSolver allows for automatic setting of nodal forces to matrix equation r.h.s.
- The name is derived from the primary variable name

 HeatSolver: Temperature Load
 FlowSolve: Flow Solution i Load
 StressSolve: Displacement i Load
 StatElecSolve: Potential Load
 ...
- Coupling between two solvers may be done either on the continuous or discrete (matrix) level
- Discrete level can often be done without any additional coding and it is at least as accurate!

 $f_{solid} = -f_{fluid}$

Test case: fsi_beam_nodalforce Setting FSI conditions on the discrete level

Displacement 1 Load = Opposes "Flow Solution Loads 1" Displacement 2 Load = Opposes "Flow Solution Loads 2"



Test case: fsi_beam Setting FSI internally on continuous level

Fsi Bc = True

Example: Dirichlet-Neumann Domain Decomposition

- Two equations for temperature: TempA and TempB
- We iterate on convergence solution such that
 Same temperatures: T_a = T_b
 Same fluxes: -kdT_a/dn = kdT_b/dn
- We use library functionalities

 Dirichlet conditions
 Computing nodal loads
 Setting nodal loads
 - Steady state iteration
 - No coding required!



CSC

Boundary Condition 3 Name = "Interface" Target Boundaries = 3

TempB = Equals TempA TempA Load = Opposes "TempB Loads" End

Periodic Boundary Conditions (node-to-surface)



• BC

Periodic BC = Integer

 Give the corresponding master boundary

 Periodic BC Varname = Logical True

 Enforce periodicity for given variable

 Periodic BC Offset Varname = Real

 Enforce desired constant offset in values

 ...

- Creates surface-to-node mapping and keeps the size of the linear system the same
- Accuracy optimal for conforming meshes only
- Accuracy not optional for non-conforming meshes

 Mortar Finite Elements

2D periodic LES simulation using VMS, by Juha Ruokolainen



Periodic BC = 2 Periodic BC Pressure = Logical True

Periodic BC Offset Pressure = Real 10.0 Periodic BC Velocity 1 = Logical True Periodic BC Velocity 2 = Logical True

Mortar Boundary conditions (surface-to-surface)



Solver

Apply Mortar BCs = Logical
 Should the solver apply the conditions?

• BC

Mortar BC = Integer

 Give the corresponding master boundary

 Galerkin Projector = Logical

 This enforces the weak projector for all dofs

 Mortar BC Static = Logical

 Projectors may be assumed to be static

0...

- Mapping of accuracy is optimal

 Adds lagrange multipliers to the system
 Convergence of linear system becomes more challenging
- Provides a framework for many complicated problems

 Rotating boundary conditions
 Contact mechanics
 Symmetric & nonconforming
- Also antiperiodic systems supported

Periodic conditions (strong): $x_l = Px_r$ Mortar conditions (weak): $Qx_l - Rx_r = 0$

Example: continuity with mortar projector in 2D

csc

• Multiple mortar BCs possible at the same time • Weights may be summed up

> Boundary Condition 6 Target Boundaries(1) = 7 Name = "Mortar Left Master" Mortar BC = Integer 7 Galerkin Projector = Logical True Plane Projector = Logical True End

```
Boundary Condition 7
Target Boundaries(1) = 6
Name = "Mortar Left Target"
End
```

test case: MortarPoisson2Dsum



Example: toy model for temperature between 2D rotor and stator



сsс

Example: Rotating 2D and 3D "machines"





CSC

51 18.3.2021



Comparison of shared boundary conditions in Elmer

BC type	Mortar BC	Periodic BC	Conforming BC
also known as	surface-to-surface	node-to-surface	elimination
Non-confoming BCs	YES	YES	NO
Matrix size	N+M	Ν	N-M
Spoils the matrix	YES	yes	NO
Edges possible	YES	NO	YES

Soft Limiters in Elmer (Inequality Constraints)

...

- General way to ensure min/max limit of solution
- A priori contact surface => soft limiters
- Uses two consepts • Nodal load evaluation
- Contact setApplicable to
 - Heat equation
 Elasticity
 Richards equation

Solver 1 Apply Limiter = True

Boundary Condition 2 Name = "Contact" Target Boundaries(1) = 6

Displacement 3 Upper Limit = Variable time Real Procedure "ContactBC" "SphereBottom" End



CSC

Hertz problem

0....

Contact mechanics in Elmer

- Utilizes the optimal mortar methods + contact sets of soft limiters
- Results to difficult linear systems • Elimination by using dual basis test functions
- Some challenges in general cases i.e. with conflicting normals



Consistency between meshes (as opposed to boundaries)

- Consistency between different meshes may only be enforced explicitely
- Mapping is done automatically when variables is needed • Octree search – optimal in speed

test case: multimesh

CSC

Boundary Condition 2 Name = "Local2Global" **Target Boundaries = 2** globalT = Equals localT End

```
localT
globalT
                                                             Triggers
                                                            mesh-to-mesh
                                                                              Boundary Condition 3
                                                            interpolation
                                                                               Name = "Global2Local"
                                                                               Target Boundaries = 3
                                                                               localT = Equals globalT
                                                                              End
```

Summary

• ~100 Solvers that try to do some specific tasks

 \circ ElmerModels Manual

- ~200,000 lines of code in the library providing a wide variety of services
 © ElmerSolver Manual
- Many undocumented features still exist!

Discussion: where to go from here?

- Current focus in Elmer/Ice and electromechanics + some smaller projects
- Architectures change as a driver

 Threading and GPU developments
 Needed to take use of supercomputers
- Open source ecosystem
 - Focus to where there software shines
 Take use of other tools when suitable -> interfaces
- Comments?

Most important Elmer resources

• <u>http://www.csc.fi/elmer</u>

 $_{\odot}$ Official Homepage of Elmer at CSC

• <u>http://www.elmerfem.org</u>

o Discussion forum, wiki, elmerice community

• <u>https://github.com/elmercsc/elmerfem</u>

GIT version control

<u>http://youtube.com/elmerfem</u>

Youtube channel for Elmer animations

- <u>http://www.nic.funet.fi/pub/sci/physics/elmer/</u>
 Download repository
- Further information: elmeradm@csc.fi

