Elmer finite element software for multiphysical problems

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ElmerTeam
CSC – IT Center for Science
Elmer track in PRACE spring school

- Wed 16th, 10.45-12.15=1.5 h
  Introduction to Elmer finite element software
- Wed 16th, 13.30-15.00=1.5 h
  Hands-on session using ElmerGUI
- Wed 16th, 15.15-16.45=1.5 h
  OpenLab
- Thu 17th, 10.45-12.15=1.5 h
  Advanced use of Elmer
- Thu 17th, 13.30-14.30=1 h
  Hands-on session on advanced features and parallel computation
- Thu 17th, 14.45-15.45=1h
  Hands-on & improvised
Elmer finite element software for multiphysical problems

Figures by Esko Järvinen, Mikko Lyly, Peter Råback, Timo Veijola (TKK) & Thomas Zwinger
Short history of Elmer

1995 Elmer development was started as part of a national CFD program
   – Collaboration of CSC, TKK, VTT, JyU, and Okmetic Ltd.

2000 After the initial phase the development driven by number of application projects
   – MEMS, Microfluidics, Acoustics, Crystal Growth, Hemodynamics, Glaciology, ...

2005 Elmer published under GPL-license

2007 Elmer version control put under sourceforge.net
   – Resulted to a rapid increase in the number of users

2010 Elmer became one of the central codes in PRACE project

2012 ElmerSolver library published under LGPL
   – More freedom for serious developers
Elmer in numbers

- ~350,000 lines of code (~2/3 in Fortran, 1/3 in C/C++)
- ~500 code commits yearly
- ~280 consistency tests in 3/2014
- ~730 pages of documentation in LaTeX
- ~60 people participated on Elmer courses in 2012
- 9 Elmer related visits to CSC in 2012
- ~2000 forum postings yearly
- ~20,000 downloads for Windows binary yearly
Elmer is published under (L)GPL

- Used worldwide by thousands of researchers (?)
- One of the most popular open source multiphysical software
~20k Windows downloads at sf.net in a year
Elmer finite element software

- **Elmer** is actually a suite of several programs
- Some components may also be used independently
- **ElmerGUI** – Preprocessing
- **ElmerSolver** – FEM Solution
  - Each physical equation is a *dynamically loaded* library to the main program
- **ElmerPost** - Postprocessing
- **ElmerGrid** – structured meshing, mesh import & partitioning
ElmerGUI

Graphical user interface of Elmer
- Based on the Qt library (GPL)
- Developed at CSC since 2/2008

Mesh generation
- Plugins for Tetgen, Netgen, and ElmerGrid
- CAD interface based on OpenCascade

Easiest tool for case specification
- Even educational use
- Parallel computation

New solvers easily supported through GUI
- XML based menu definition

Also postprocessing with VTK
ElmerPost

- Developed in late 90’s by Juha Ruokolainen at CSC
- All basic presentation types
  - Colored surfaces and meshes
  - Contours, isosurfaces, vectors, particles
  - Animations
- Includes MATC language
  - Data manipulation
  - Derived quantities
- Output formats
  - ps, ppm, jpg, mpg
  - Animations
- Largely replaced by Paraview
ElmerGrid

- Creation of 2D and 3D structured meshes
  - Rectangular basic topology
  - Extrusion, rotation
  - Simple mapping algorithms

Mesh Import
- About ten different formats:
  - Ansys, Abaqus, Fidap, Comsol, Gmsh,...

Mesh manipulation
- Increase/decrease order
- Scale, rotate, translate

Partitioning
- Simple geometry based partitioning
- Metis partitioning
  Example: > ElmerGrid 1 2 step -metis 10

Usable via ElmerGUI
- All features not accessible (partitioning, discont. BC,...)
ElmerSolver

- Assembly and solution of the finite element equations
- Many auxiliary routines
- Good support for parallelism

Note: When we talk of Elmer we mainly mean ElmerSolver

> ElmerSolver StepFlow.sif
MAIN: ==================================================
MAIN:  E L M E R  S O L V E R  S T A R T I N G
MAIN:  Library version: 5.3.2
MAIN: ==================================================
MAIN:  
MAIN:  
MAIN:  -----------------------
MAIN:  Reading Model ...
...

SolveEquations: (NRM,RELC): ( 0.34864185 0.88621713E-06 ) :: navier-stokes
: *** Elmer Solver: ALL DONE ***
SOLVER TOTAL TIME(CPU,REAL): 1.54 1.58
ELMER SOLVER FINISHED AT: 2007/10/31 13:36:30
ElmerSolver – Finite element shapes

- 0D: vertex
- 1D: edge
- 2D: triangles, quadrilateral
- 3D: tetrahedrons, prisms, pyramids, hexahedrons
ElmerSolver – Finite element basis functions

- **Element families**
  - nodal, DG
  - p-elements
  - edge, face – elements
    - $H_{\text{div}}$ (often associated with "face" elements)
    - $H_{\text{curl}}$ (often associated with "edge" elements)

- **Formulations**
  - Galerkin, Discontinuous Galerkin
  - Stabilization
  - Residual free bubbles
ElmerSolver – meshing features

- Internal mesh multiplication

- Internal mesh extrusion

- Discontinuities
  - Mortar finite elements for periodic and conforming/nonconforming meshes
  - Creation of discontinuities at selected boundaries

- Adaptivity
  - For selected equations
  - no parallel implementation
ElmerSolver – Time dependency modes

- Steady-state simulation
- Transient simulation
  - 1st order PDEs:
    - Backward differences formulae (BDF) up to 6th degree
    - Cranck-Nicolsen
  - 2nd order PDEs:
    - Bossak
- Harmonic simulation
- Eigenmode simulation
  - Utilizes (P)Arpack library
- Scanning
  - Special mode for parametric studies etc.
ElmerSolver – Linear solvers

- Iterative Krylov subspace methods
  - HUTiter library (part of Elmer)
  - Optional: Trilinos (Belos) & Hypre

- Multigrid methods
  - AMG (serial only) and GMG included in Elmer
  - Optional: Hypre/BoomerAMG and Trilinos/ML

- Preconditioners
  - ILU, BILU, multigrid, SGS, Jacobi,…
  - Generic block preconditioning
  - Optional: Hypre (Parasails, ILU), Trilinos

- FETI
  - PCG+MUMPS
  - Optional: Flophy (VSB)

- Direct solvers
  - Lapack (banded), Umfpack
  - Optional: SuperLU, MUMPS, Pardiso
Poll on application fields (status 3/2014)

What are your main application fields of Elmer?

<table>
<thead>
<tr>
<th>Field</th>
<th>Votes</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat transfer</td>
<td>64</td>
<td>28%</td>
</tr>
<tr>
<td>Fluid mechanics</td>
<td>61</td>
<td>27%</td>
</tr>
<tr>
<td>Solid mechanics</td>
<td>47</td>
<td>21%</td>
</tr>
<tr>
<td>Electromagnetics</td>
<td>38</td>
<td>17%</td>
</tr>
<tr>
<td>Quantum mechanics</td>
<td>3</td>
<td>1%</td>
</tr>
<tr>
<td>Something else (please specify)</td>
<td>12</td>
<td>5%</td>
</tr>
</tbody>
</table>

Total votes: 225

Submit vote
Elmer – Heat Transfer

- Heat equation
  - convection
  - diffusion
  - Phase change
  - Temperature control feedback
  - Thermal slip BCs for small Kn number

- Radiation with view factors
  - 2D, axisymmetric use numerical integration
  - 3D based on ray tracing
  - Stand-alone program

- Strongly coupled thermoelectric equation

- Associated numerical features
  - Steady state, transient
  - Stabilization, VMS
  - ALE

- Typical couplings
  - Mesh movement
  - Electricity - Joule heating
  - Fluid - convection

- Known limitations
  - Turbulence modeling not extensively validated
  - ViewFactor computation not possible in parallel
Microfluidics: Flow and heat transfer in a microchip

- Electrokinetically driven flow
- Joule heating
- Heat Transfer influences performance
- Elmer as a tool for prototyping
- Complex geometry
- Complex simulation setup

Elmer – Fluid Mechanics

- Navier-Stokes (2D & 3D)
  - Nonnewtonian models
  - Slip coefficients
- RANS turbulence models
  - $SST \; k-\Omega$
  - $k-\varepsilon$
  - $\nu^2-f$
- Large eddy simulation (LES)
  - Variational multiscale method (VMS)
- Reynolds equation
  - Dimensionally reduced N-S equations for small gaps (1D & 2D)

- Associated numberical features
  - Steady-state, transient
  - Stabilization
  - ALE formulation
- Typical couplings
  - FSI
  - Thermal flows (natural convection)
  - Transport
  - Free surface
  - Particle tracker

- Known limitations
  - Only experimental segregated solvers
  - Stronger in the elliptic regime of N-S i.e. low Re numbers
  - RANS models have often convergence issues
Czockralski Crystal Growth

- Most crystalline silicon is grown by the Czochralski (CZ) method
- One of the key applications when Elmer development was started in 1995


Figures by Okmetic Ltd.
CZ-growth: Transient simulation

Parallel simulation of silicon meltflows using stabilized finite element method (5.4 million elements).

Simulation Juha Ruokolainen, animation Matti Gröhn, CSC
Glaceology

- **Elmer/Ice** is the leading software used in 3D computational glaciology
- Full 3D Stokes equation to model the flow
- Large number of tailored models to deal with the special problems
- Motivated by climate change and sea level rise
- Dedicated community portal [elmerice.elmerfem.org](http://elmerice.elmerfem.org)

Thermal creep in light mills

2D compressible Navier-Stokes eq. with heat eq. plus two rarefied gas effects:

- Maxwell’s wall slip and thermal transpiration

\[
    u_x(I) = \frac{2 - \sigma}{\sigma} \lambda \left( \frac{\partial u_x}{\partial n} + \frac{\partial u_n}{\partial x} \right) + \frac{3\mu}{4\rho T} \frac{\partial T}{\partial x}
\]

- Smoluchowski’s temperature jump

\[
    T_G - T_W = \frac{2 - \sigma_T}{\sigma_T} \frac{2\gamma}{\gamma + 1} \frac{\lambda}{Pr} \frac{\partial T}{\partial n}
\]

Moritz Nadler, Univ. of Tuebingen, 2008
VMS turbulence modeling

- Large eddy simulation (LES) provides the most accurate presentation of turbulence without the cost of DNS.
- Requires transient simulation where physical quantities are averaged over a period of time.
- Variational multiscale method (VMS) by Hughes et al. Is a variant of LES particularly suitable for FEM.
- Interaction between fine (unresolved) and coarse (resolved) scales is estimated numerically.
- No ad hoc parameters.

Plane flow with $\Re_\tau = 395$
Elmer – Solid mechanics

- Linear elasticity (2D & 3D)
  - Linear & orthotropic material law
  - Thermal and residual stresses
- Non-linear Elasticity (in geometry)
  (unisotropic, lin & nonlin)
  - Neo hookean material law
- Plate equation
  - Spring, damping
- Shell equation
  - Undocumented

Associated numerical features
- Steady-state, harmonic, eigenmode
- Simple contact model

Typical physical coupling
- Fluid-Structure interaction (FSI)
- Thermal stresses
- Source for acoustics

Known limitations
- Limited selection of material laws
- Only simple contact model
MEMS: Inertial sensor

- MEMS provides an ideal field for multi-physical simulation software
- Electrostatics, elasticity and fluid flow are often inherently coupled
- Example shows the effect of holes in the motion of an accelerometer prototype

Figure by VTI Technologies

Elasticity – von Mises stresses

http://www.studiogarattoni.com/
Cardiovascular diseases are the leading cause of deaths in western countries.

Calcification reduces elasticity of arteries.

Modeling of blood flow poses a challenging case of fluid-structure-interaction.

Artificial compressibility is used to enhance the convergence of FSI coupling.

Elmer – Electromagnetics

- StatElecSolve for insulators
  - Computation of capacitance matrix
  - Dielectric surfaces
- StatCurrentSolve for conductors
  - Computation of Joule heating
  - Beedback for desired heating power
- Magnetic induction
  - Induced magnetic field by moving conducting media (silicon)
- MagnetoDynamics2D
  - Applicable also to rotating machines
- MagnetoDynamics3D
  - Modern AV formulation utilizing edge-elements
  - Steady-state, harmonic, transient

- Associated numerical features
  - Mainly formulations based on scalar and vector potential
  - Lagrange elements except mixed nodal-edge elements for AV solver
- Typical physical couplings
  - Thermal (Joule heating)
  - Flow (plasma)
  - Rigid body motion
- Known limitations
  - Limited to low-frequency (small wave number)
  - One needs to be weary with the Coulomb gauge in some solvers
AV solver for magnetic fields

Simulation by "madstamm"
In elmerfem.org/forum,
11/2011
Simulation of Welding

Simulation by Alessandro Rovera, Bitron, Italy, 2014.
Simulation of electrical machines

New developments in edge element basis and rotating boundary conditions enable simulation of electrical machines

*Magnetic field strength (left) and electric potential (right) of an electrical engine end-windings. Meshing M. Lyly, ABB. Simulation J. Ruokolainen, CSC, 2013.*

Elmer – other physical models

- Species transport
- Groundwater flow, Richards equation
- DFT, Kohn-Sham equations
- Iter reactor, fusion plasma equilibrium
- Optimization
- Particle tracking
- ...
Quantum Mechanics

- Finite element method is used to solve the Kohn-Sham equations of density functional theory (DFT)
- Charge density and wave function of the 61st eigenmode of fullerene C60
- All electron computations using 300,000 quadratic tets and 400,000 dofs

Simulation Mikko Lyly, CSC, 2006
Optimization in FSI

Elmer includes some tools that help in the solution of optimization problems.

Profile of the beam is optimized so that the beam bends as little as possible under flow forces.

Optimized profiles for $Re=\{0, 10, 50, 100, 200\}$

Pressure and velocity distribution with $Re=10$

Simulation Peter Råback, CSC
Particle tracker - Granular flow

Simulation Peter Råback, CSC, 2011.
Elmer – Selected multiphysics features

Solver is an abstract dynamically loaded object
- Solver may be developed and compiled without touching the main library
- No upper limit to the number of Solvers (Currently ~50)

Solvers may be active in different domains, and even meshes
- Automatic mapping of field values

Parameters of the equations are fetched using an overloaded function allowing
- Constant value
- Linear or cubic dependence via table
- Effective command language (MATC)
- User defined functions with arbitrary dependencies
- As a result solvers may be weakly coupled without any \textit{a priori} defined manner

Tailored methods for some difficult strongly coupled problems
- Consistant modification of equations (e.g. artificial compressibility in FSI, pull-in analysis)
- Monolitic solvers (e.g. Linearized time-harmonic Navier-Stokes)
Solution strategies for coupled problems

Hierarchical solution

Iterative solution

Monolithic solution
Possible reasons for using Elmer (or Open Source software in general)
Reasons to use open source software in CE
free as in "beer" vs. free as in "speech"

- New algorithms
- New equations
- Collaboration
- Software development
- Large scale comp. science
- Parallelism
- License costs
Savings from license costs

- A common motivation for using OS software
  - As the only reason may result to disappointment
- If the software is not previously familiar the learning curve with OS software may be quite long
- Will the marginal utility of the work with the people doing the analysis be acceptable with OS software?
  - Requires often more versatile IT skills
- Typically license cost is an issue for smaller company (or team)
- When the number of parallel licences grow the problem of license costs may become relevant also for bigger companies
Benefits of the openness of the code

- In collaboration all parties have access to the software
  - Companies, universities, consultants,…

- Open source software has more different roles
  - May be used to attract a wider spectrum of actors

- Also fundamental ideas may be tested with the software
  - Algorithms, models,…
  - Compatible with scientific method: falsification

- More possibilities to built tailored solutions
  - OS codes have usually good extendability & customizability

- At least some control over the intellectual property
  - Own model development does not become a hostage to vendor lock in
  - Sometimes rules GPL licence out of question
Generic benefits of open source software

**GBDirect** "Benefits of Using Open Source Software"

1. Reliability
2. Stability
3. Auditability
4. Cost
5. Flexibility and Freedom
6. Support and Accountability

**PCWorld** "10 Reasons Open Source Is Good for Business"

1. Security
2. Quality
3. Customizability
4. Freedom
5. Flexibility
6. Interoperability
7. Auditability
8. Support Options
9. Cost
10. Try Before You Buy
Usability vs. Extendability

Generally commercial tools are easier to use

However there is a caveat

- GUI (or a closed interface) can never be exhaustive
- “making most of the things simple makes some of the things much harder”

In open source tools you have basically access to all data and also can often utilize well defined APIs

- Extending beyond current capabilities is often more realistic & faster
- Open source software need not to be considered fixed in terms of capabilities, you can always code new stuff...
Open source software in computational engineering

- Academicly rooted stuff is top notch
  - Linear algebra, solver libraries
  - PetSc, Trilinos, OpenFOAM, LibMesh++, ...

- CAD and mesh generation not that competitive
  - OpenCASCADE legacy software
  - Mesh generators netgen, tetgen, Gmsh are clearly academic
  - Also for OpenFOAM there is development of commercial preprocessing tools

- Users may need to build their own workflows from the most suitable tools
  - Also in combination with commercial software
  - Excellent libraries for software development (Qt, python,...)
Weaknesses of OS software in CE

**CAD & Meshing**
- There is no process that would bring the best software under open source

**Lack of standardization**
- Bottom-up type (Bazaar) of open source projects seem fundamentally incompatible with ISO 9001 standard
- One should perhaps not design buildings using OS software for the computation...

**Big business**
- There are no global service organization for OS software (except maybe for OpenFOAM)
- The information management of CAD and simulation data is becoming an integral part of the work flow in large businesses and currently OS does not have solutions for that (?)
Use cases of OS software in industry

- Small consultancy or high-tech company
  - Skilled labour takes most out of OS software without license constraints

- Company with academic collaboration
  - Open Source software enables study of novel problems and attracts also scientifically minded students

- Company with in-house simulation development
  - Open Source tools may provide optimal steps in internal workflow development

- Company with pursuing HPC
  - Good scalability without license constraints
Elmer – Infrastructure for Open Research

Elmer As Infrastructure

- Elmer Courses
- Elmer Support
- GPL modules
- propriety modules
- HPC
- Elmer Library

University D
Institute C
Company B
User / Developer / Customer
Most important Elmer resources

- [http://www.csc.fi/elmer](http://www.csc.fi/elmer)
  - Official Homepage of Elmer
- [http://sourceforge.net/projects/elmerfem/](http://sourceforge.net/projects/elmerfem/)
  - Version control system & Windows binaries
- [www.elmerfem.org](http://www.elmerfem.org)
  - Discussion forum, wiki & doxygen

Further information: elmeradm@csc.fi

Thank you for your attention!