Elmer
Open Source Finite Element Software for Multiphysical Problems

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CSC – IT Center for Science

PATC course on parallel workflows
Stockholm, 4-6.12.2013
What is CSC?

- Founded in 1971 as a technical support unit for Univac 1108
- Connected Finland to the Internet in 1988
- Reorganized as a company, CSC – Scientific Computing Ltd. in 1993
- All shares to the Ministry of Education and Culture of Finland in 1997
- Operates on a non-profit principle
- Facilities in Espoo, close to Otaniemi campus and Kajaani
- Staff ~200
- Turnover 2009 21,9 million euros
- Currently official name is: "CSC – IT Center for Science Ltd."
The volume of data is growing exponentially. To exploit the data for, e.g., drug design, a global, constantly updating IT infrastructure is needed (programs, DBs).
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
Developers of Elmer

Current developers at CSC
- Core Elmer team: Mika Malinen, Juha Ruokolainen, Peter Råback, Thomas Zwinger
- Accentional developers: Mikko Byckling, Sampo Sillanpää, Sami Ilvonen

Other/past developers & contributors
- CSC: Mikko Lyly, Erik Edelmann, Jussi Heikonen, Esko Järvinen, Jari Järvinen, Antti Pursula, Ville Savolainen,, ...
- VTT: Martti Verho
- TKK: Jouni Malinen, Harri Hakula, Mika Juntunen
- Trueflaw: Iikka Virkkunen
- Open Innovation: Adam Powell
- LGGE: Olivier Gagliardini, Fabien Gillet-Chaulet,...
- University of Uppsala: Jonas Thies
- etc... (if your name is missing, please ask it to be added)
Elmer in numbers

- ~500 code commits yearly
- ~230 consistency tests in 4/2013
- ~350,000 lines of code (~2/3 in Fortran, 1/3 in C/C++)
- ~730 pages of documentation in LaTeX
- ~4 FTs used with about half in projects in 2012
- ~60 people participated on Elmer courses in 2013
- 9 Elmer related visits (1 week-2 months) to CSC in 2013
- ~2000 forum postings yearly
- ~20,000 downloads for Windows binary in 2013
- ~50% of CSC’s web page traffic
Elmer is published under (L)GPL

- Used worldwide by thousands of researchers (?)
- Perhaps the most popular open source multiphysical software targeted to end-users
- ~20,000 Windows binary downloads 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
SERIAL WORKFLOW: VISUALIZATION
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: 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
ElmerPost

- Has roots in the FUNCS program
  - written in late 80’s and early 90’s by Juha Ruokolainen
- 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
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,...)
Core features of ElmerSolver

Physical Models
- Fluid mechanics
- Structural mechanics
- Electromagnetics
- Acoustics
- Heat transfer
- Mass transport
- Free surface problems
- Particle tracking
- Quantum mechanics
- ...

Numerical Methods
- Time dependency: steady, transient, harmonic, eigenmode
- Large selection of element types (nodal, edge, face, p-elements)
- Several stabilization methods
- Large selection of direct, iterative and multigrid linear solvers
- Fully supported parallelism
Elmer technical highlights

- A unique modular structure that enables versatility in multiphysics even for end-user
- High level of abstraction – physics neutral library
- MPI parallelism inherently built-in
- Early adaptor in advanced features
  - Iterative methods ~1997
  - GMG & mesh multiplication ~2003
  - Adaptivity ~2004
  - Block preconditioning 2010
  - FETI ~2011
  - Ported on Intel MICs 2012
  - Mortar finite elements for rotating problems 2013
  - ...
Poll on application fields (status 10/2013)

What are your main application fields of Elmer?

You may select up to 5 options

<table>
<thead>
<tr>
<th>Field</th>
<th>Votes</th>
<th>Percentage</th>
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<td>Heat transfer</td>
<td>63</td>
<td>29%</td>
</tr>
<tr>
<td>Fluid mechanics</td>
<td>59</td>
<td>27%</td>
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<tr>
<td>Solid mechanics</td>
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<tr>
<td>Electromagnetics</td>
<td>38</td>
<td>17%</td>
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<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>
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Total votes: 221

[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 – 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

Elmer – Fluid Mechanics

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

- Associated numerical 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
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
Czochralski Crystal Growth

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

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
MEMS – Perforated plates

- Modified Reynolds equations may be used to model squeezed film pressure under perforated plates
- Comparison with very heavy 3D computations show good agreement (see figure)

Simulation: Timo Veijola
Thermal creep in light mills

- Glass container in a very low pressure < 10 Pa
- Each ving has a black and silver side
- When hit by light the light mill rotates with silver side ahead

The physical explanation of the light mills requires consideration of rarefied gases and thermal creep

These were studied in the thesis project of Moritz Nadler, University of Tubingen, 2008
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

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

- Smoluchowski’s temperature jump

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

Simulation Moritz Nadler, 2008
Computational Hemodynamics

- 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
  - Feedback for desired heating power
- Magnetic induction
  - Induced magnetic field by moving conducting media (silicon)
- Magnetostatics (old)
  - Axisymmetric solver for Joule heating
- MagnetoDynamics2D
  - Rotating machines
- MagnetoDynamics3D
  - AV formulation
  - 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
Scalability of Whitney element AV solver for end-windings

Magnetic field strength (left) and electric potential (right) of an electrical engine end-windings. Meshing M. Lyly, ABB. Simulation (Cray XC, Sisu) J. Ruokolainen, CSC, 2013.
Electric machine: Mortar finite elements

- Continuity of results between stator and rotor is ensured by mortar finite element technique
- Technique is applicable also to periodic systems

Model specification Antero Arkkio, Meshing Paavo Rasilo, Aalto Univ.
Simulation Juha Ruokolainen, CSC
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
Iter fusion reactor

- Assumption that 2D dependencies are valid also on a perturbed 3D system
- 3D magnetic fields but no real plasma simulation

Simulation Peter Råback, CSC, 2013
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 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)
Elmer – Infrastructure for Open Research

Elmer Courses
Elmer Support
GPL modules
propriety modules
Elmer Library
HPC

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

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

Further information: elmeradm@csc.fi

Thank you for your attention!