Elmer

Open Source Finite Element Software for Multiphysical Problems

Peter Råback, D.Sc.

ElmerTeam

CSC – IT Center for Science

Elmer/Ice advanced course

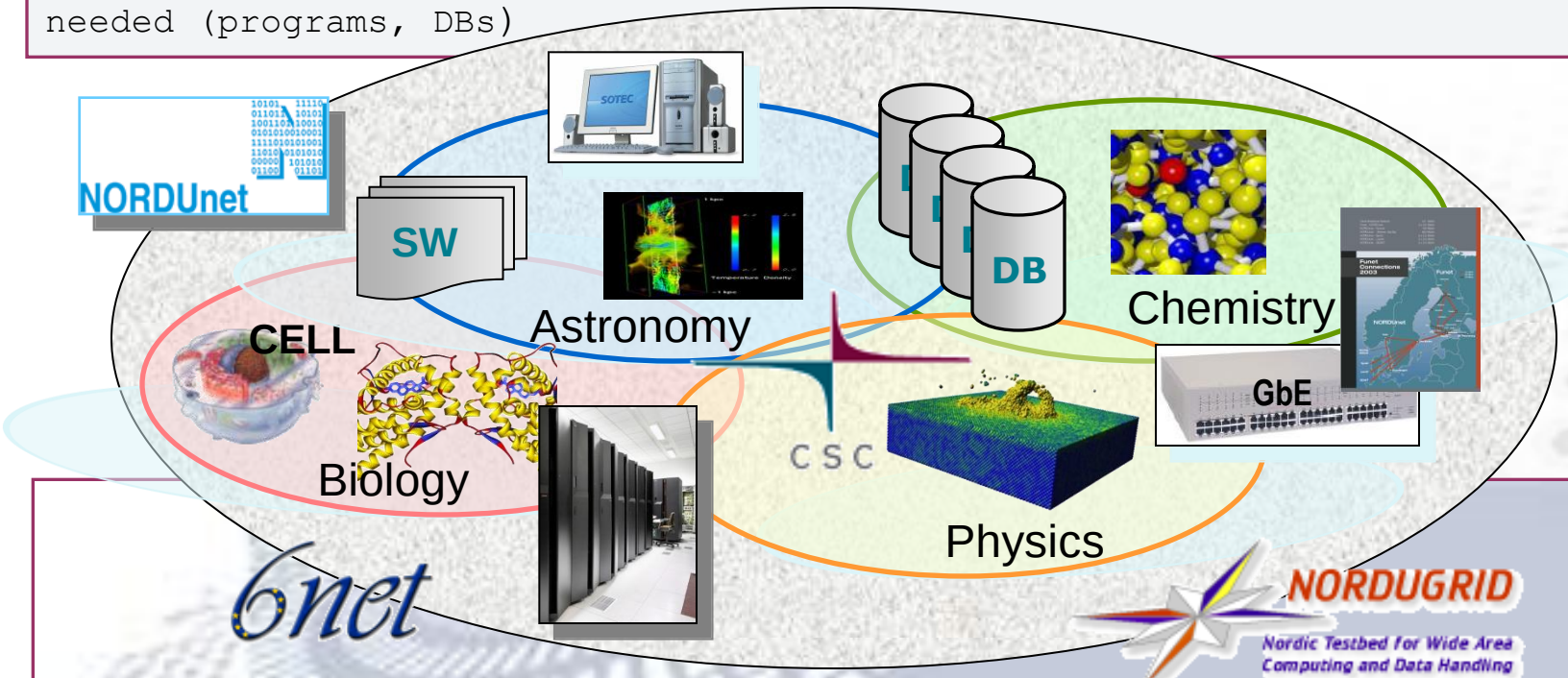
CSC, 4-6.11.2013

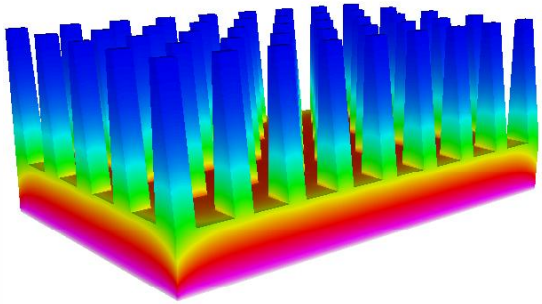
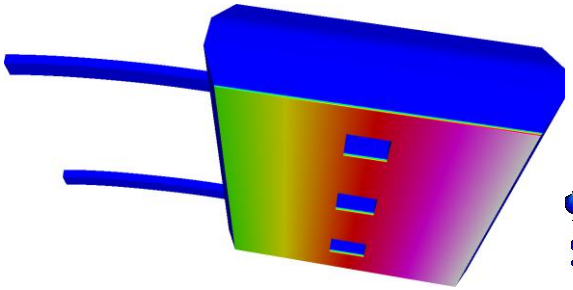
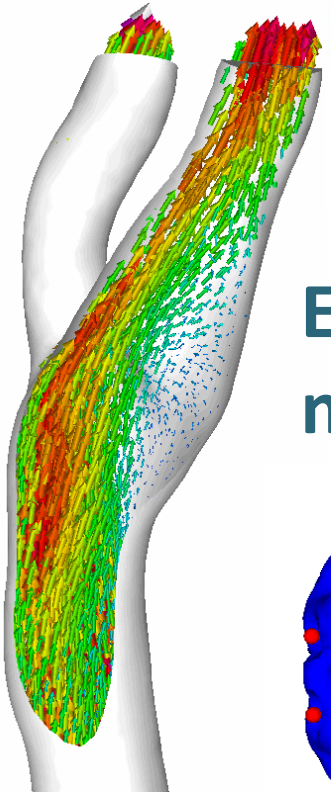
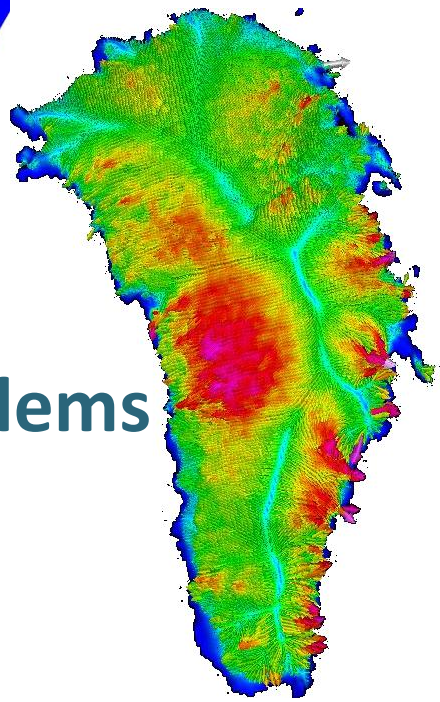
What is CSC?

- 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.”**

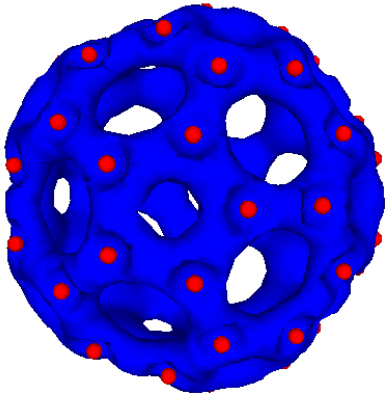
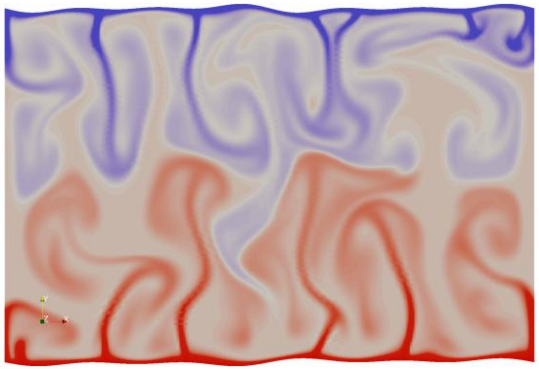
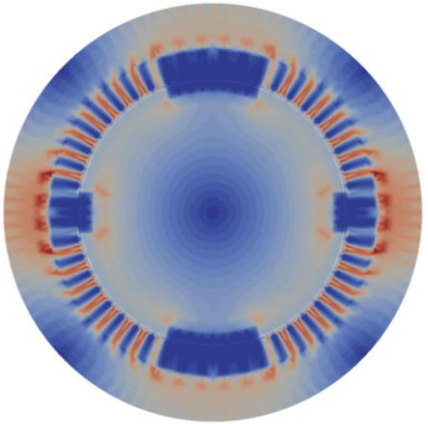
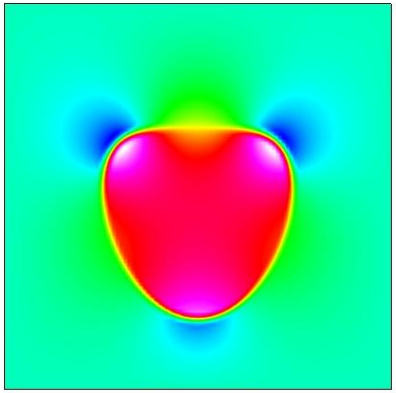
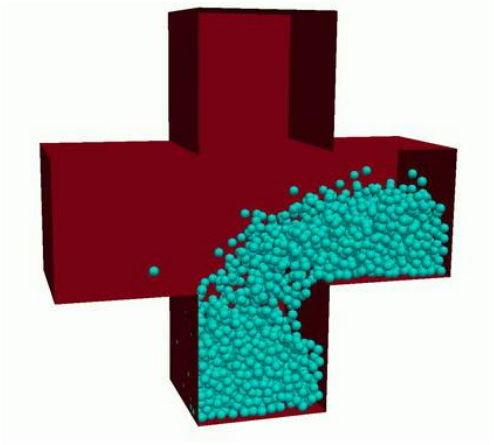
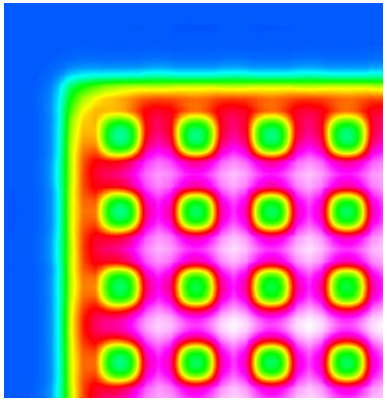
CSC as a Finnish IT Infrastructure for Research

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 and multiscale 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 to be published under LGPL
  - More freedom for serious developers

Developers of Elmer

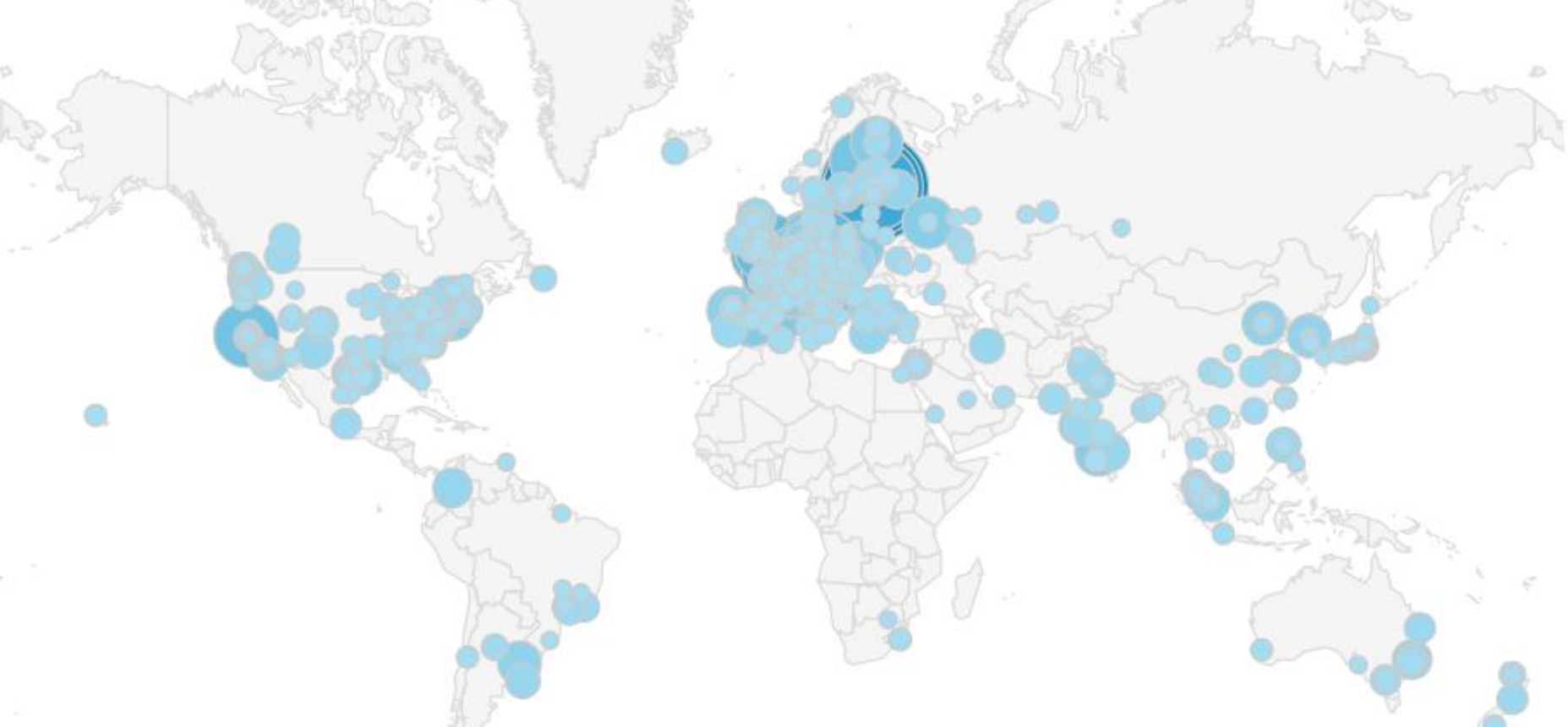
- Current developers at CSC
  - Core Elmer team: Mika Malinen, Juha Ruokolainen, Peter Råback, Thomas Zwinger
  - Accational developers: Mikko Byckling, Sampo Sillanpää, Sami Ilvonen
- Other/past developers & contributors
  - CSC: Mikko Lyly, Erik Edelmann, Jussi Heikonen, Esko Järvinen, Jari Järvinen, 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 (1week-2months) to CSC in 2013
- ~2000 forum postings yearly
- ~20,000 downloads for Windows binary in 2013
- ~50% of CSC's web page traffic

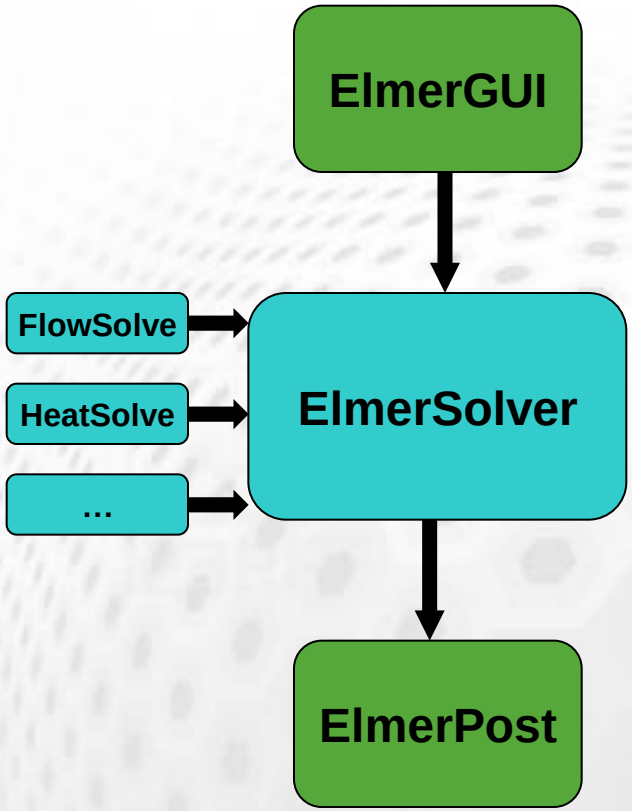
Elmer is published under (L)GPL

- 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



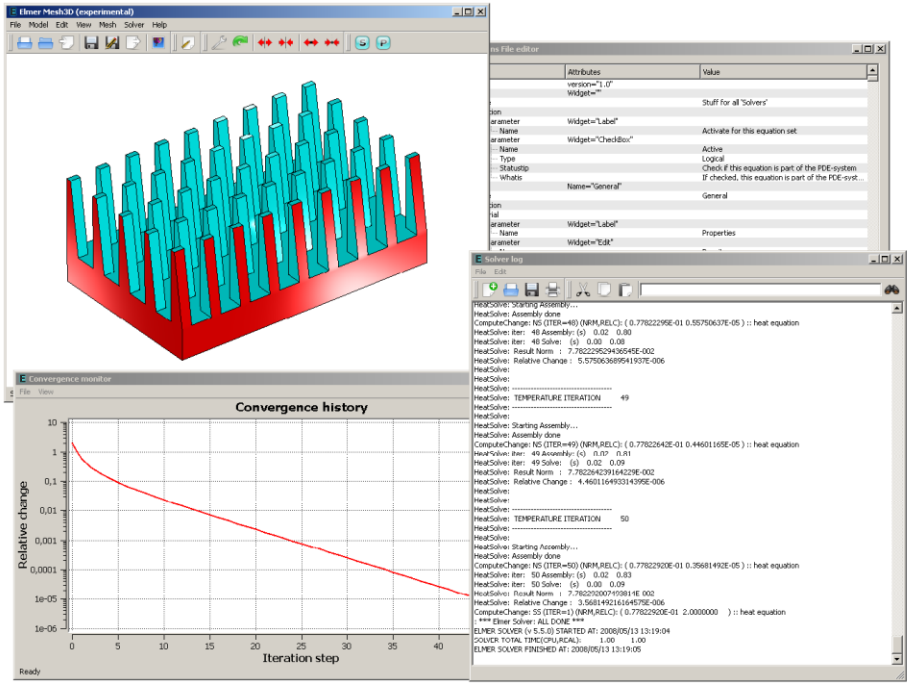
Elmer finite element software

- **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

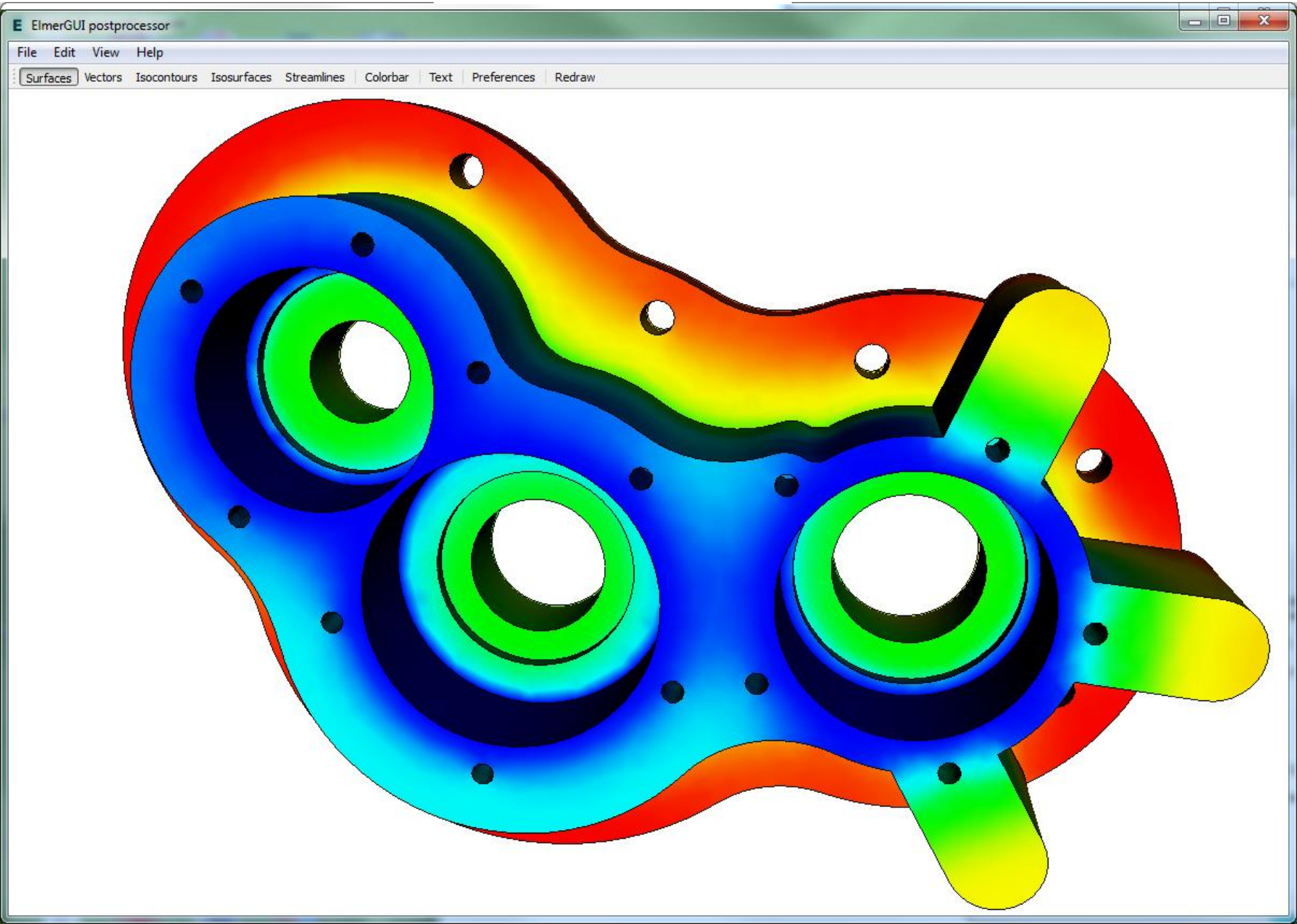


ElmerGUI

- 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



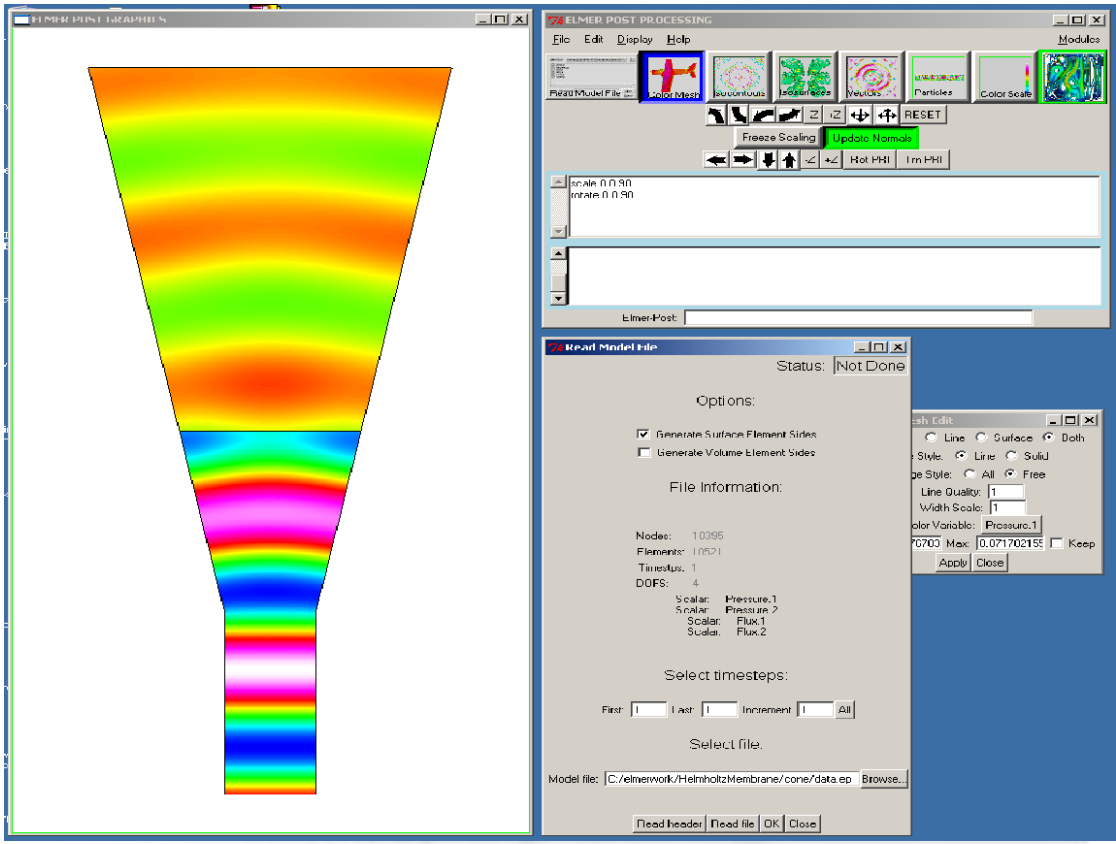
ElmerSolver

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

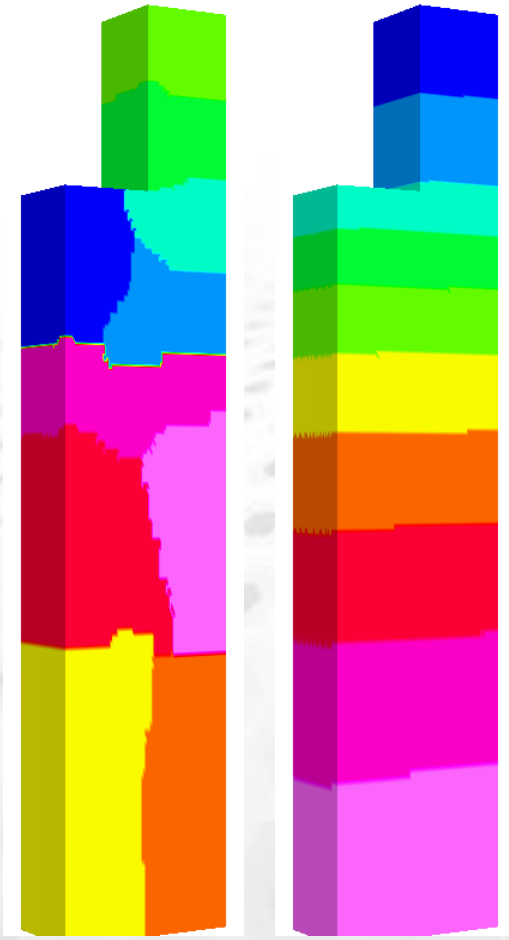
ElmerPost

- 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 algorhitms
- 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
- …

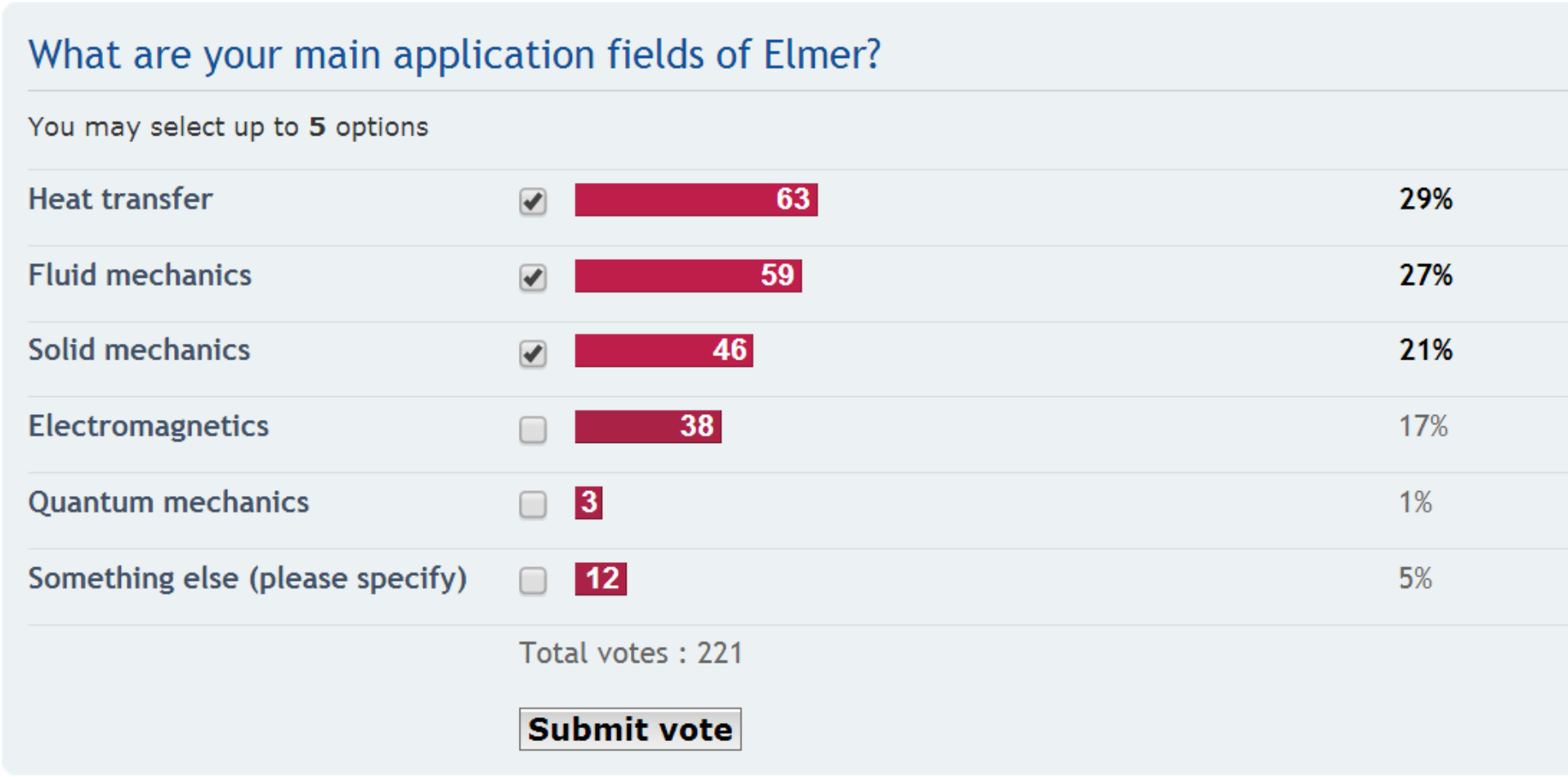
Numerical Methods

- 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 parallellism

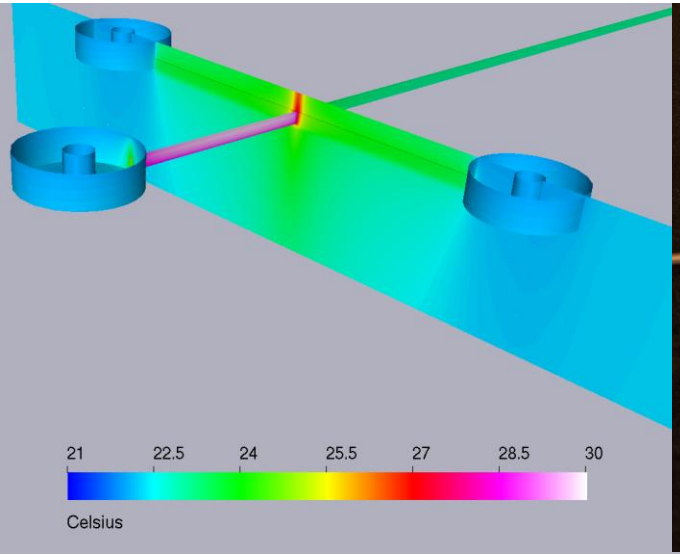
Elmer technical highligths

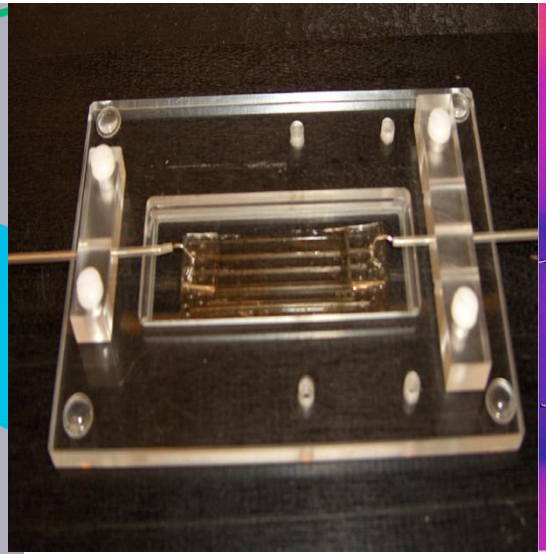
- A unique modular structure that enables versatility in multiphysics even for end-user
- High level of abstraction – physics neutral library
- MPI parallelism inherently built-in
- Early adaptor in advanced features
  - Iterative methods ~1997
  - GMG & mesh multiplication ~2003
  - Adaptivity ~2004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

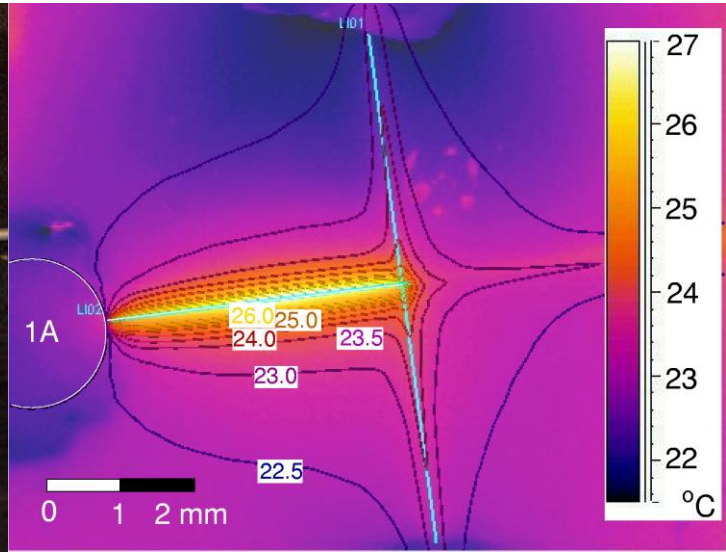
Poll on application fields (status 10/2013)



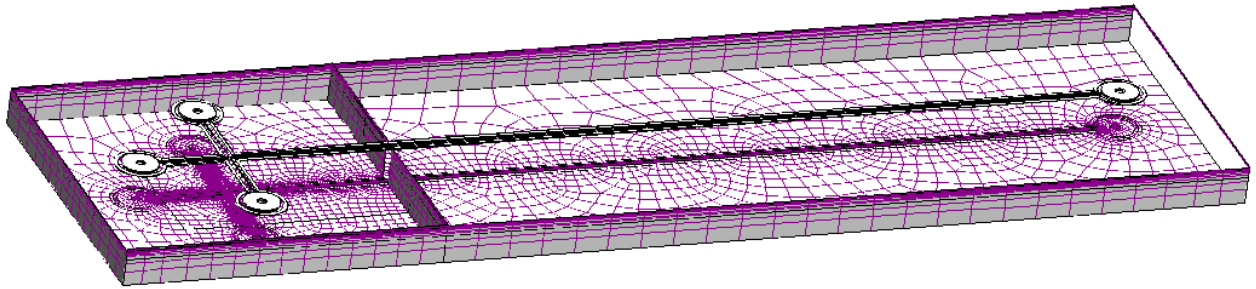
Microfluidics: Flow and heat transfer in a microchip







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



T. Sikanen, T. Zwinger, S. Tuomikoski, S. Franssila, R. Lehtiniemi, C.-M. Fager, T. Kotiaho and A. Pursula,
Microfluidics and Nanofluidics (2008)

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

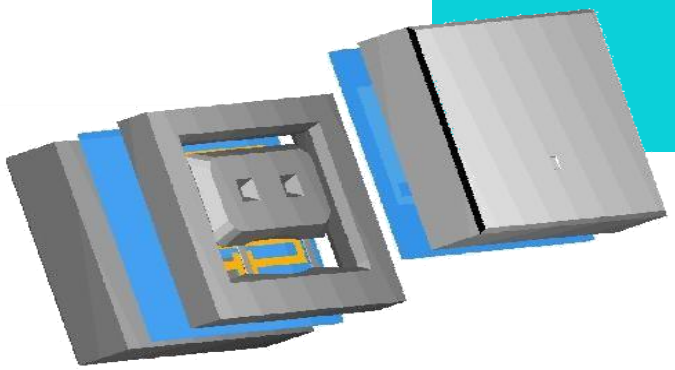
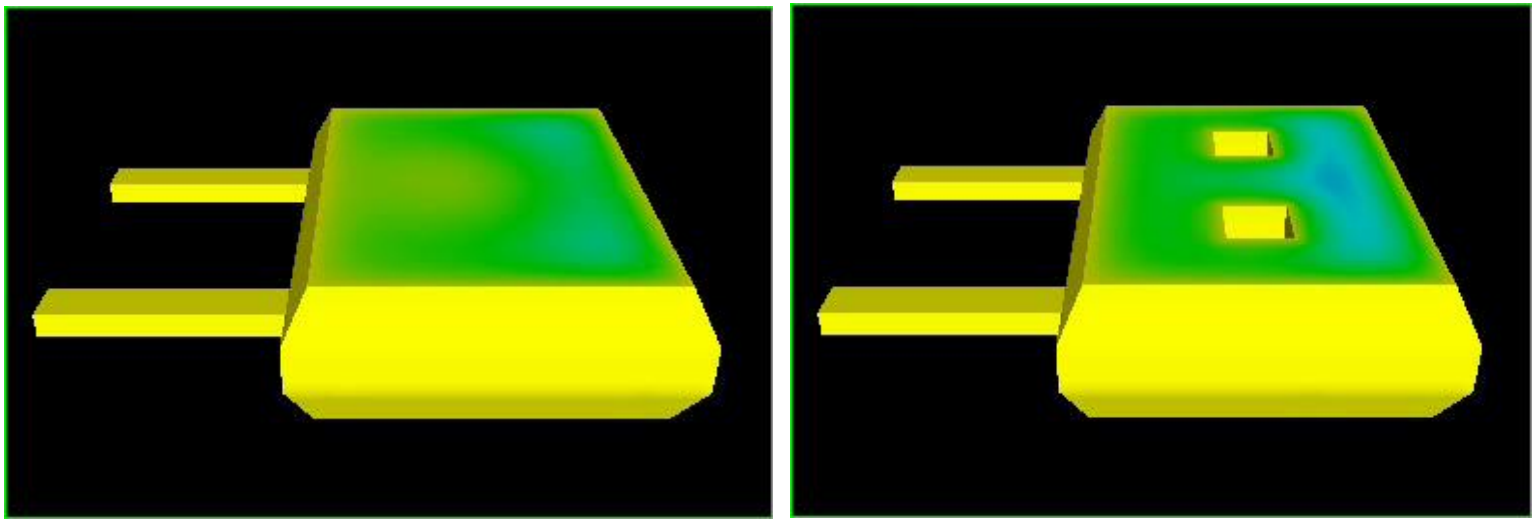


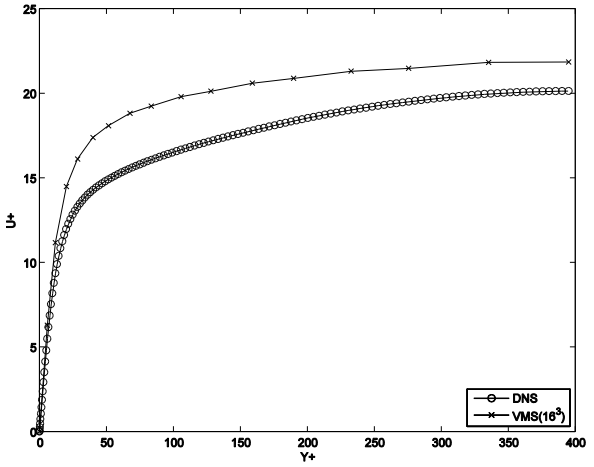
Figure by VTI Technologies



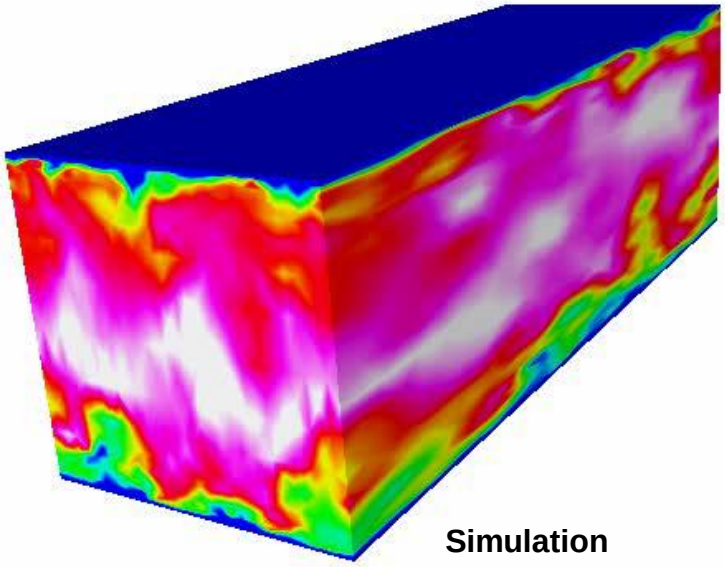
A. Pursula, P. Råback, S. Lähteenmäki and J. Lahdenperä, *Coupled FEM simulations of accelerometers including nonlinear gas damping with comparison to measurements*,
J. Micromech. Microeng. **16** (2006), 2345-2354.

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
- Interation between fine (unresolved) and coarse (resolved) scales is estimated numerically
- No ad'hoc parameters



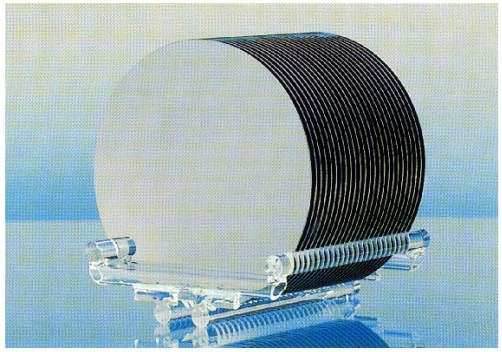
Plane flow with Re_τ=395



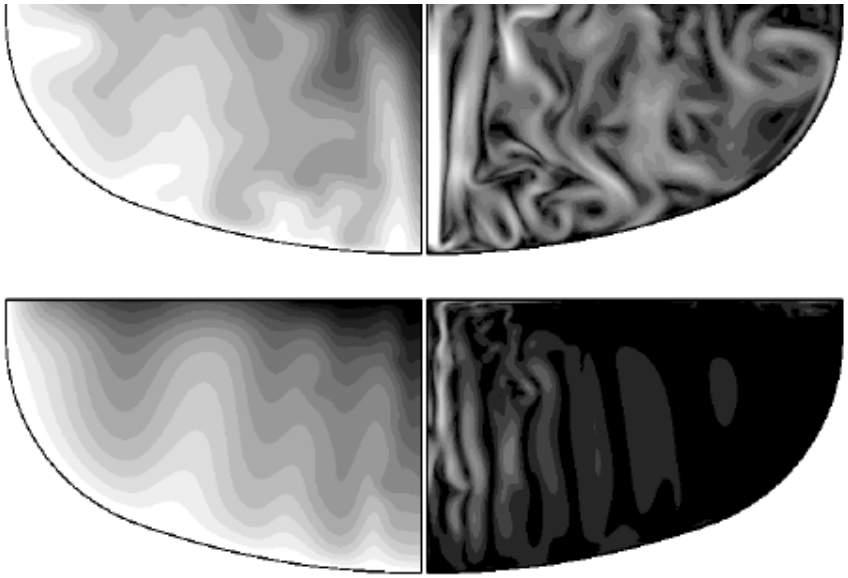
Simulation
J. Ruokolainen, CSC

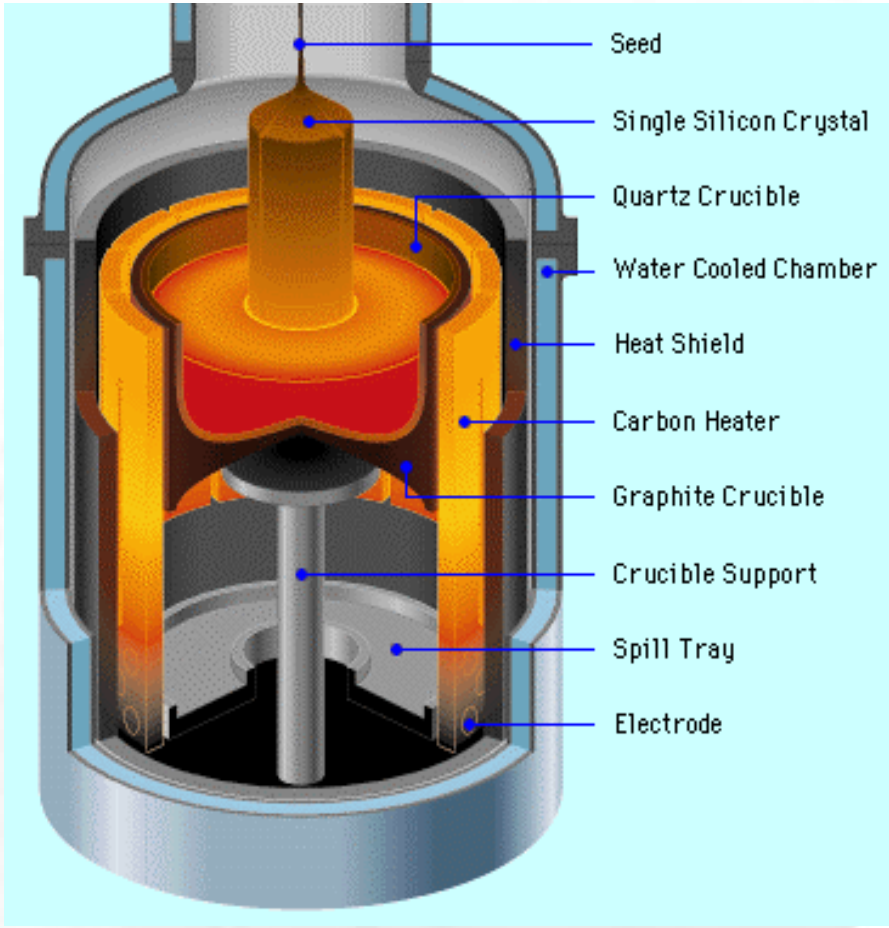
Czockralski Crystal Growth

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



Figures by Okmetic Ltd.



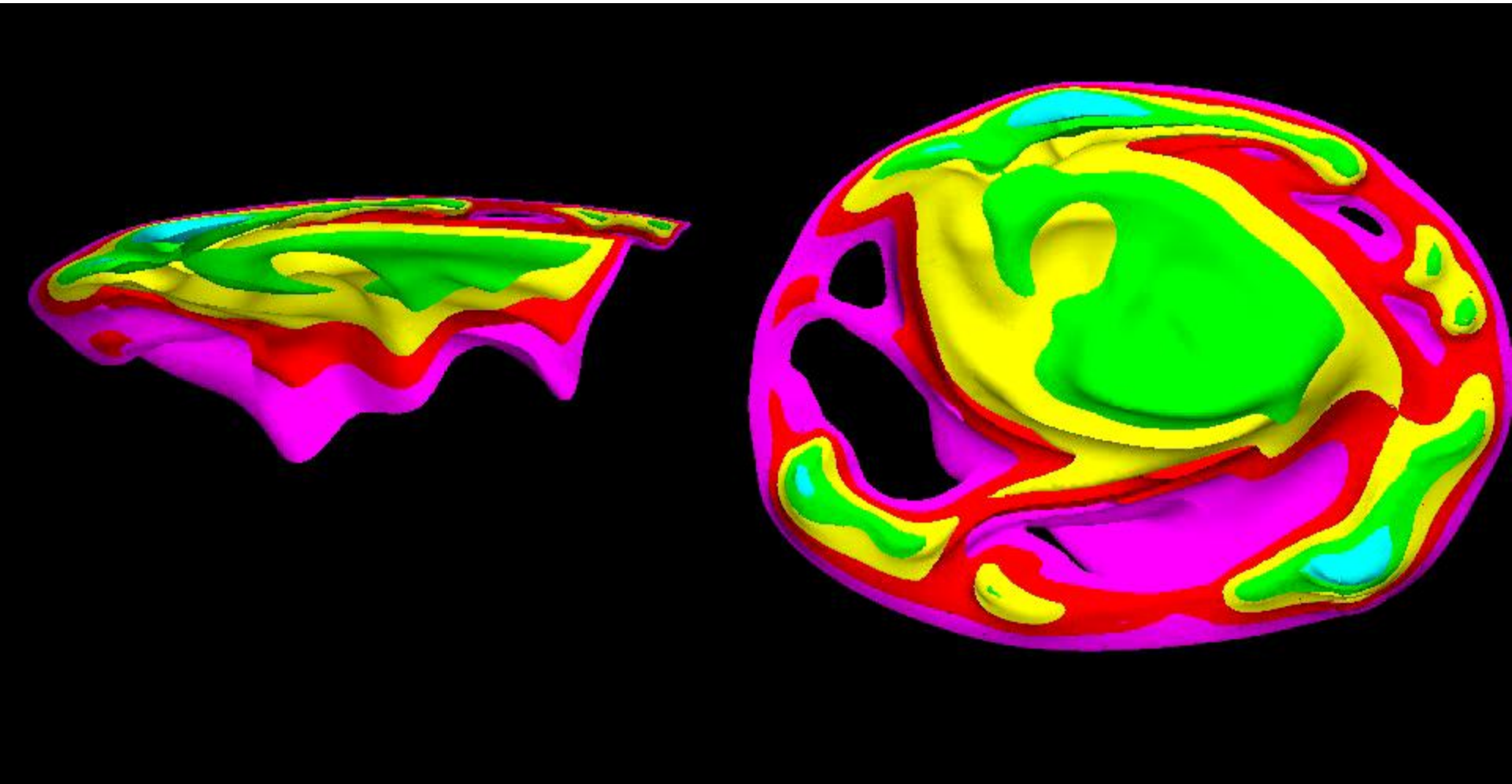


V. Savolainen et al., *Simulation of large-scale silicon melt flow in magnetic Czochralski growth,* J. Crystal Growth 243 (2002), 243-260.

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

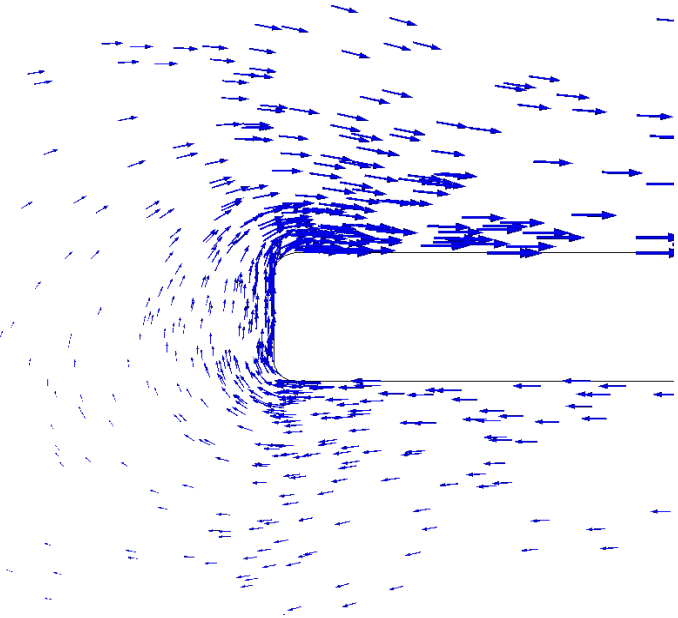


Thermal creep in light mills

- 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



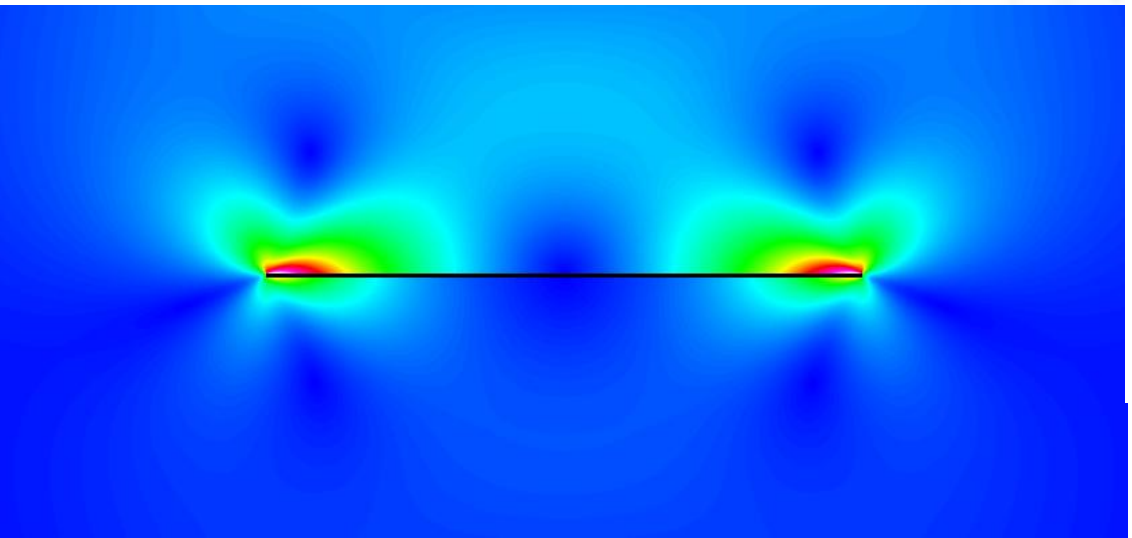
2D compressible Navier-Stokes eq. with heat eq. plus two rarefied gas effects:

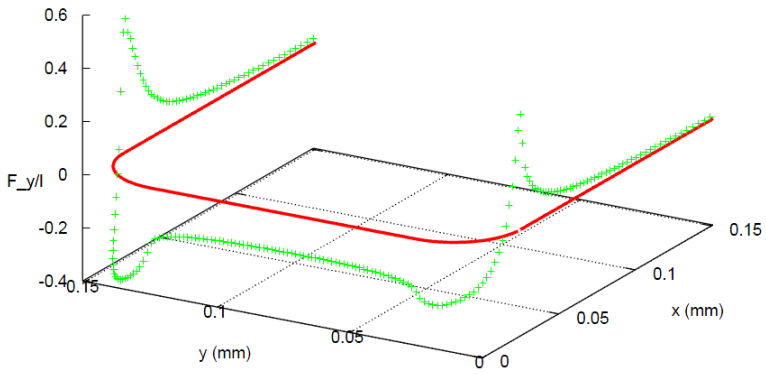
- Maxwell's wall slip and thermal transpiration

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

- Smoluchowski's temperature jump

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

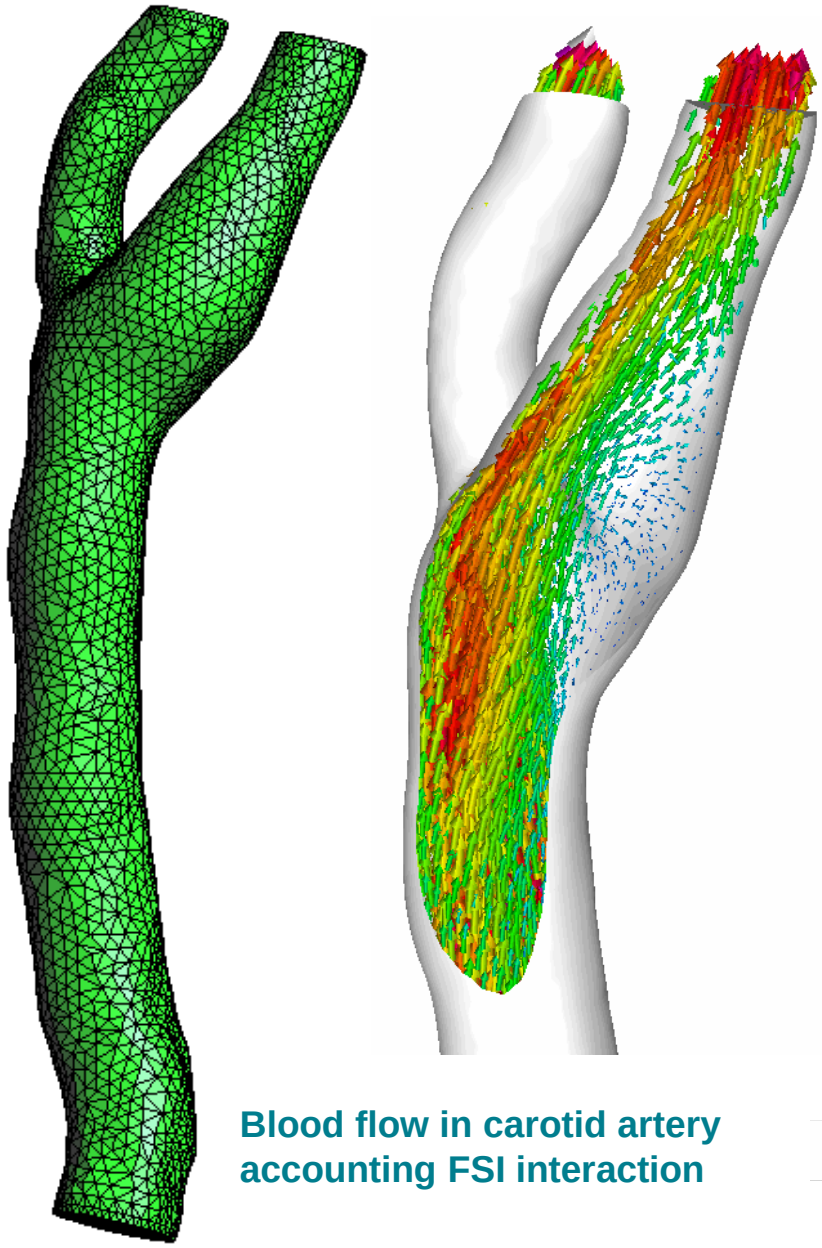




Simulation Moritz Nadler, 2008

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



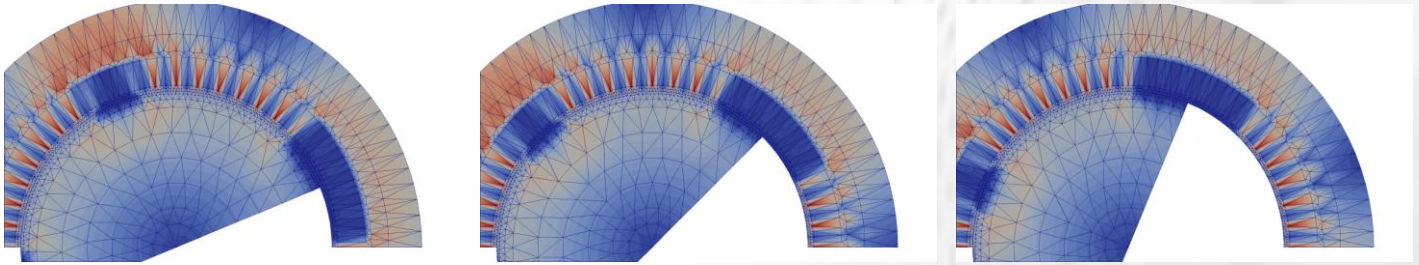
Blood flow in carotid artery accounting FSI interaction

E. Järvinen, P. Råback, M. Lyly, J. Salonius. *A method for partitioned fluid-structure interaction computation of flow in arteries. Medical Eng. & Physics*, **30** (2008), 917-923

Simulation of electrical machines

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

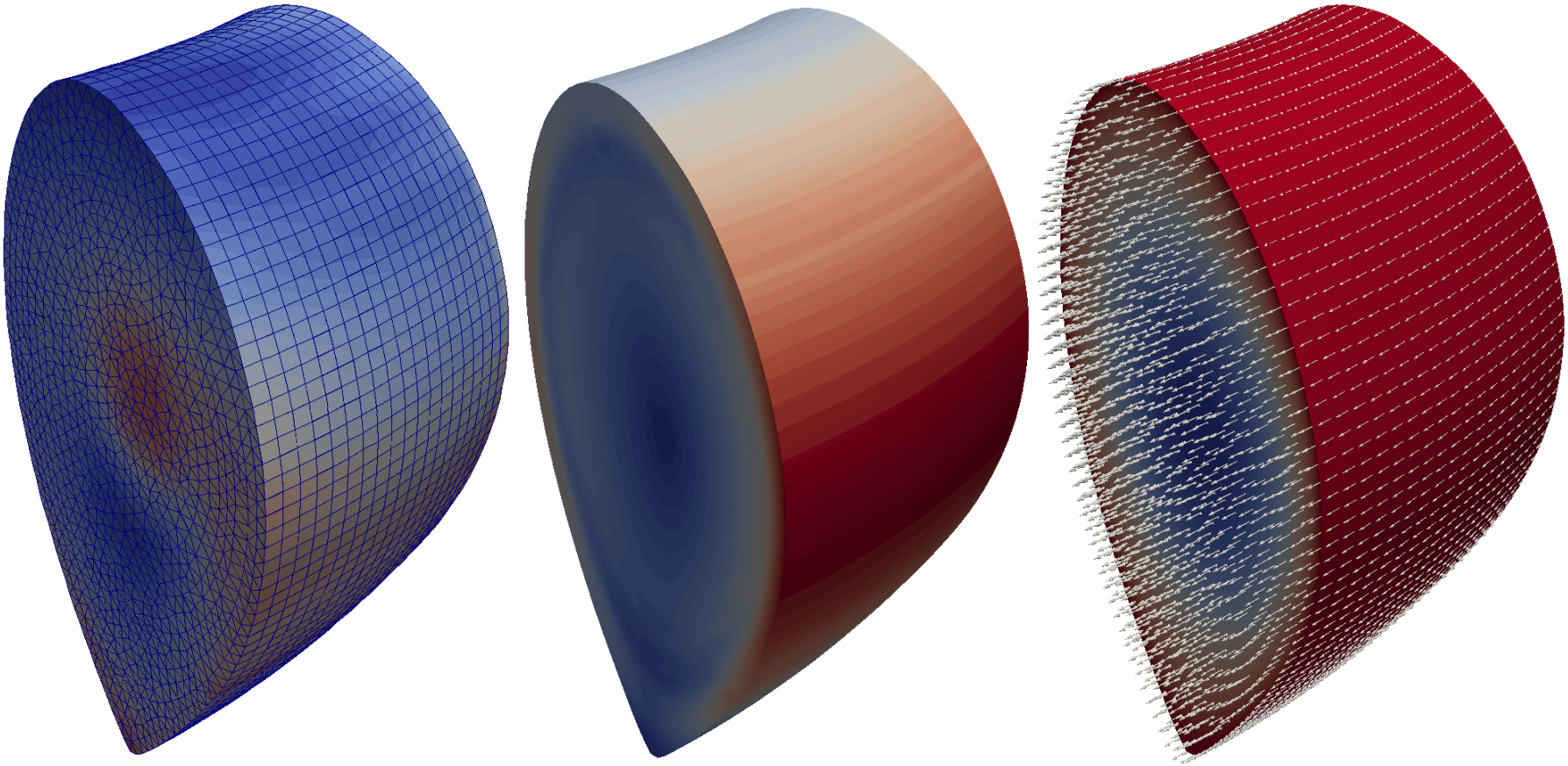
Magnetic field strength (left) and electric potential (right) of an electrical engine end-windings. Meshing M. Lyly, ABB. Simulation J. Ruokolainen, CSC, 2013.



Model specification Antero Arkkio, Meshing Paavo Rasilo, Aalto Univ.
Simulation Juha Ruokolainen, CSC, 2013.

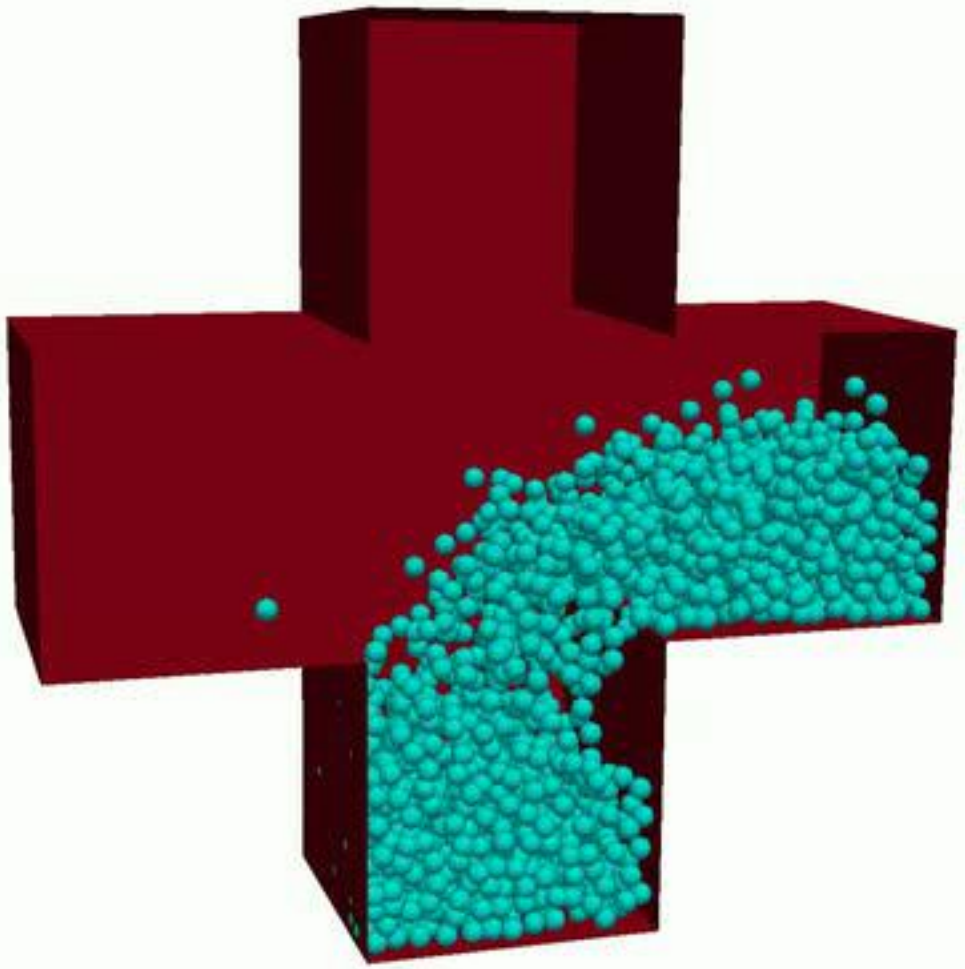
Iter fusion reactor

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



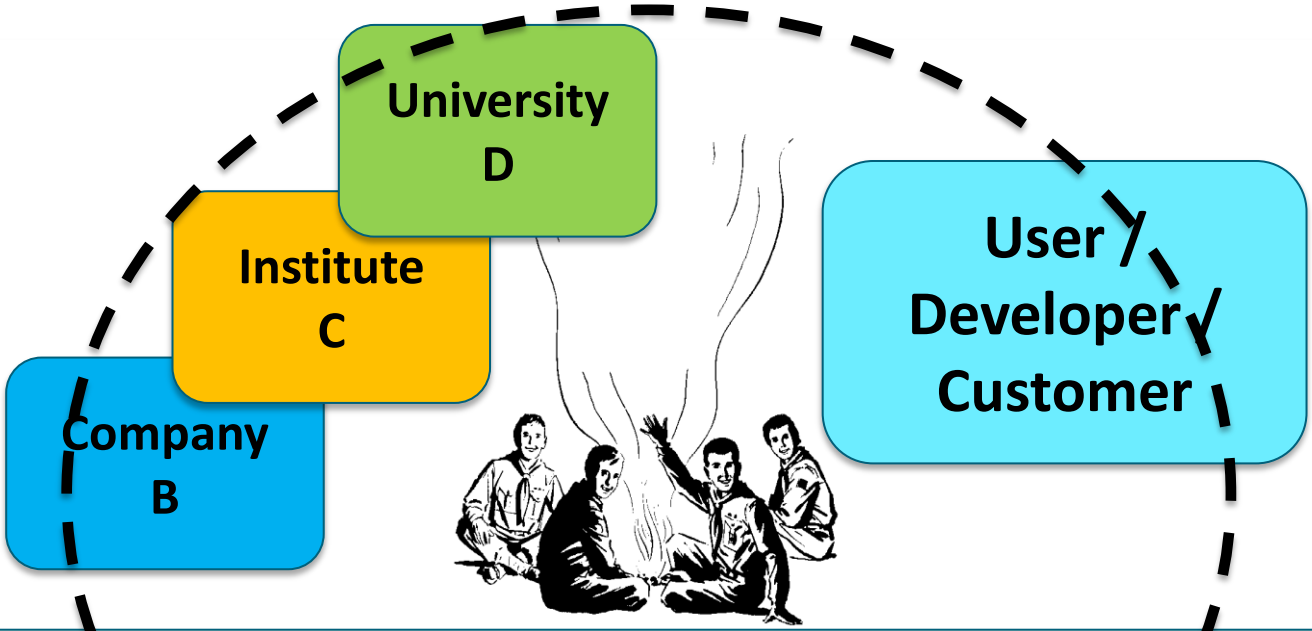
Simulation Peter Råback, CSC, 2013

Particle tracker - Granular flow

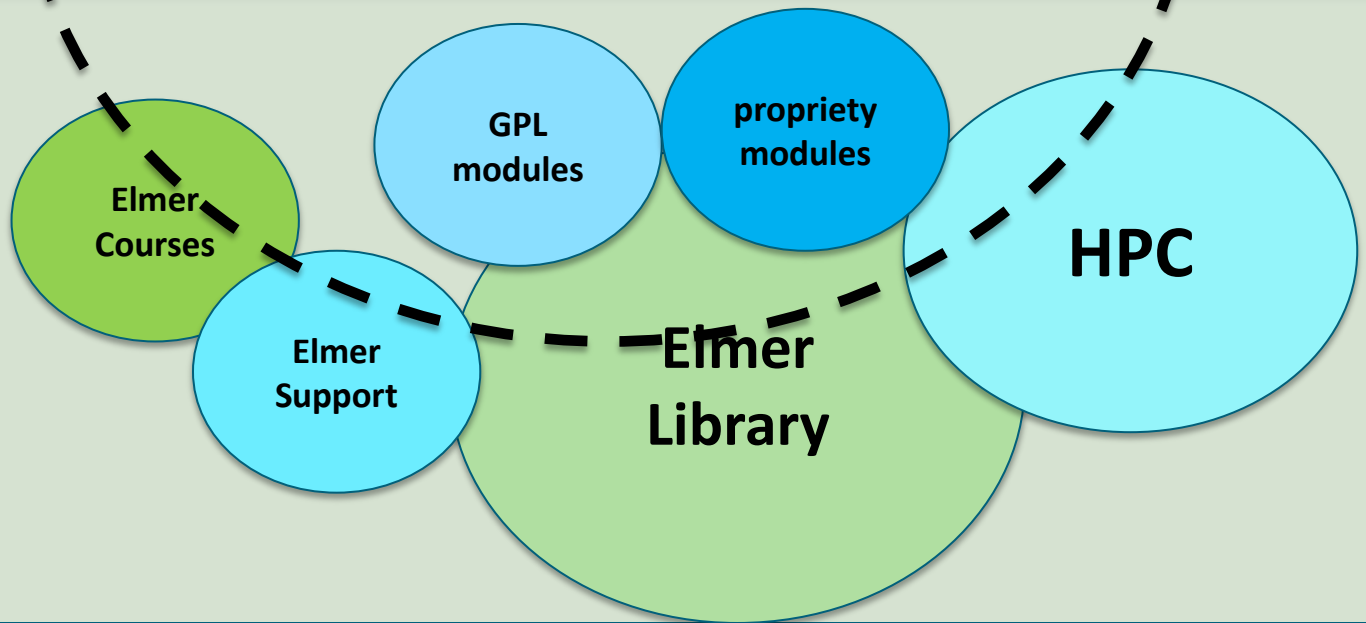


Simulation Peter Råback, CSC, 2011.

Elmer – Infrastructure for Open Research



Elmer As Infrastructure



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!