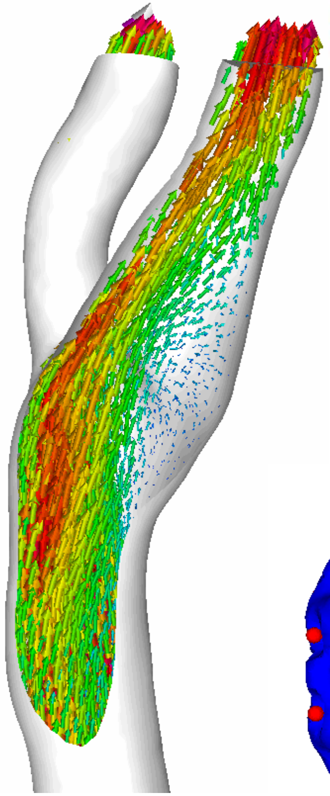
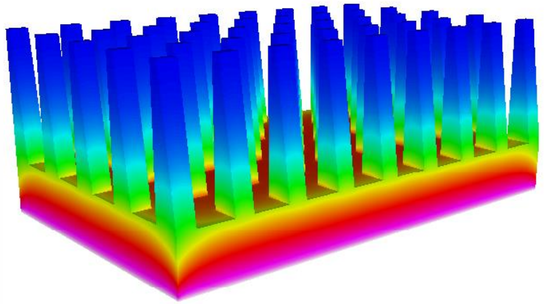
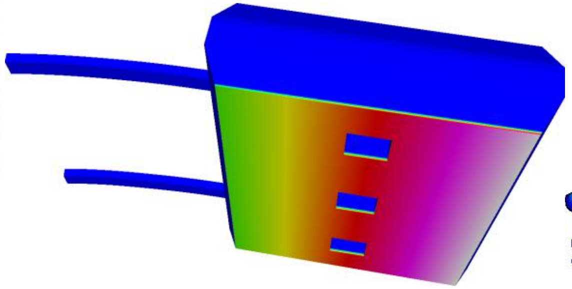
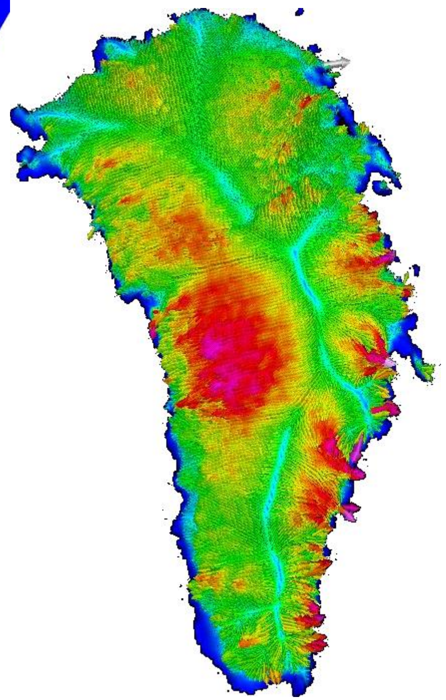
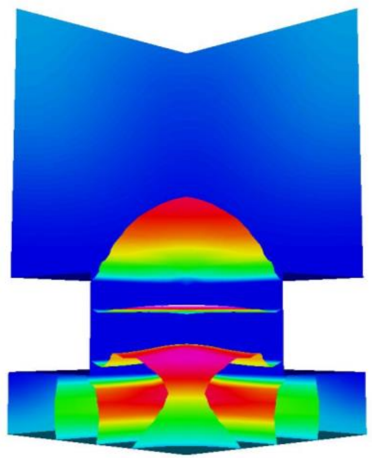
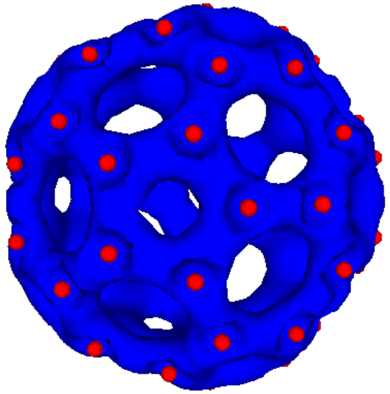
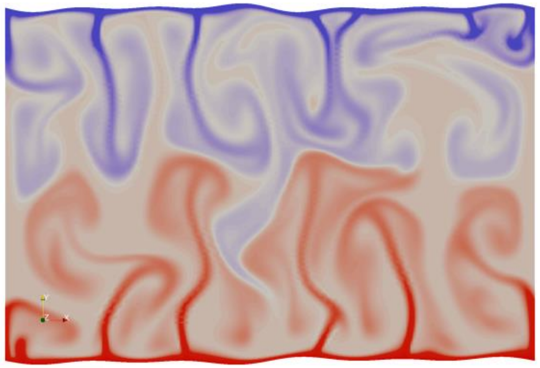
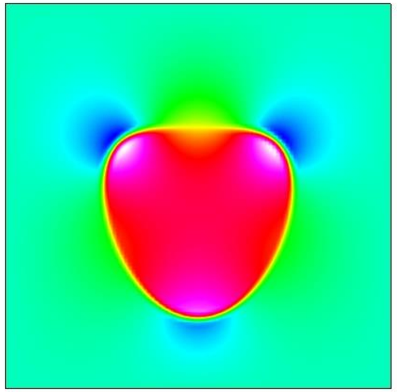
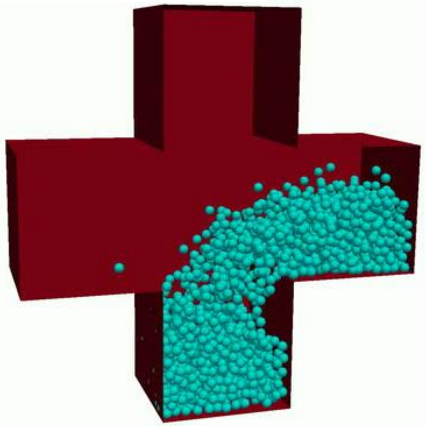
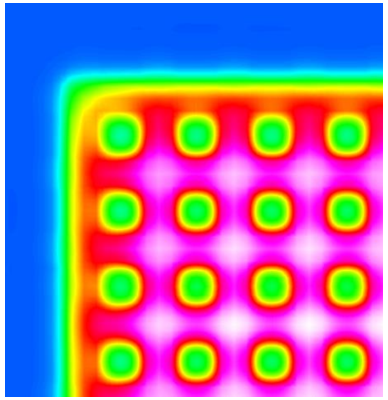
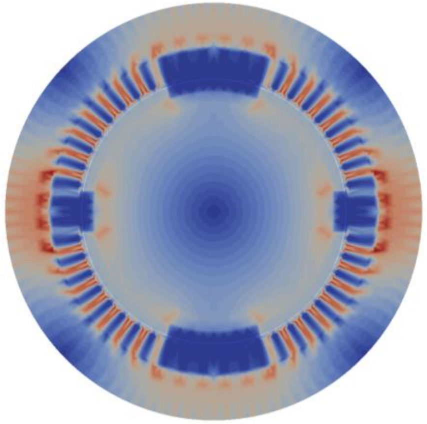
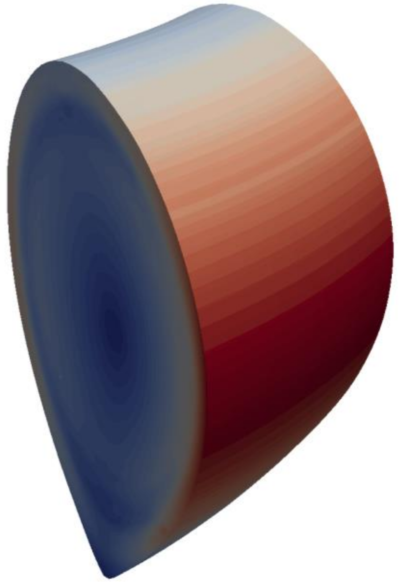
Introduction to Elmer FEM software

ElmerTeam
CSC – IT Center for Science, Finland

CSC, 2020

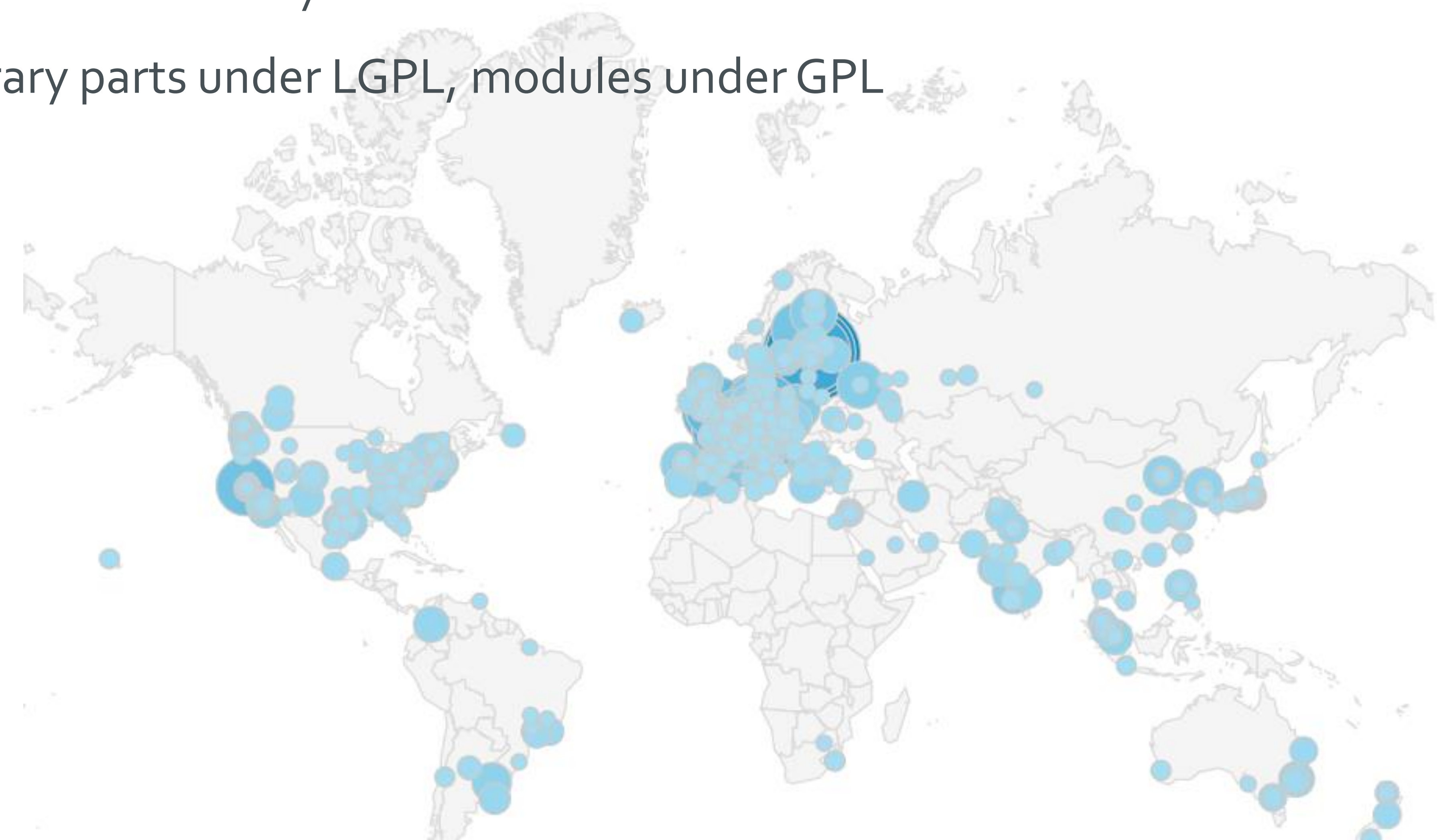
Elmer finite element software for multiphysical problems

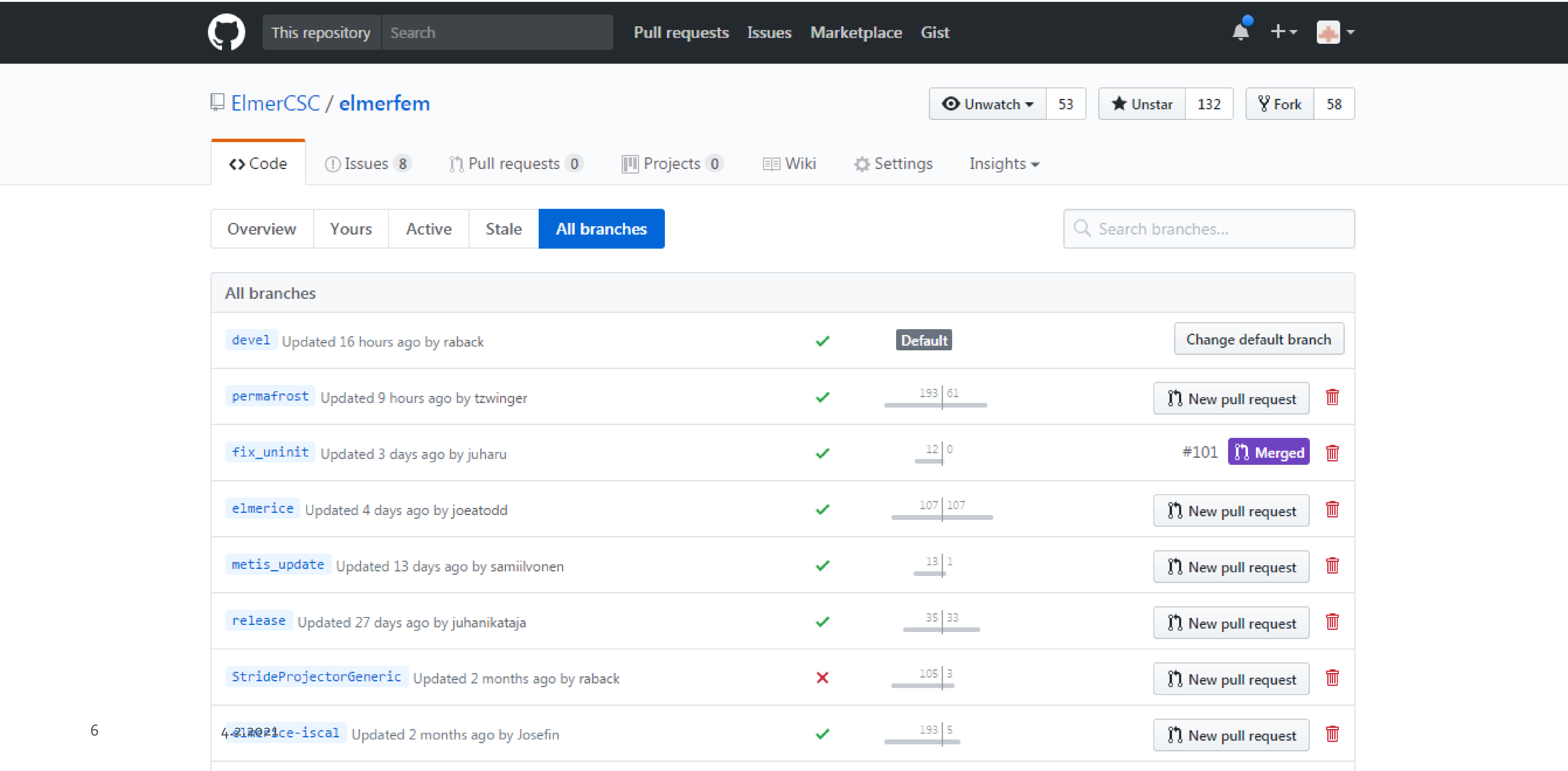
Figures by Esko Järvinen, Mikko Lyly, Peter Råback, Timo Veijola (TKK) & Thomas Zwinger

Elmer was published under open source in 2008

- Used worldwide by thousands of researchers
- Library parts under LGPL, modules under GPL



Elmer is hosted at GitHub and accepts contributions



Elmer in numbers

Software

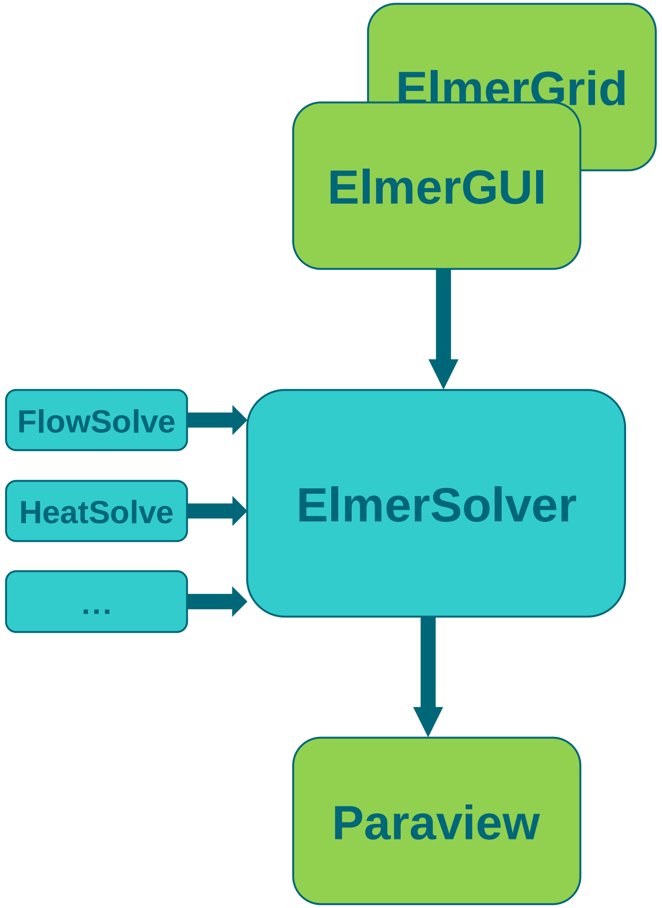
- ~400,000 lines of active code
  - ~3/4 in Fortran, 1/4 in C/C++
- ~700 consistency tests
- ~750 pages of documentation
- ~1000 code commits yearly

Community

- ~20,000 downloads for Windows binary yearly
  - Linux users untracked
- ~2000 forum postings yearly
- ~100 people participate on Elmer courses yearly
- Several Elmer related scientifc visits to CSC yearly

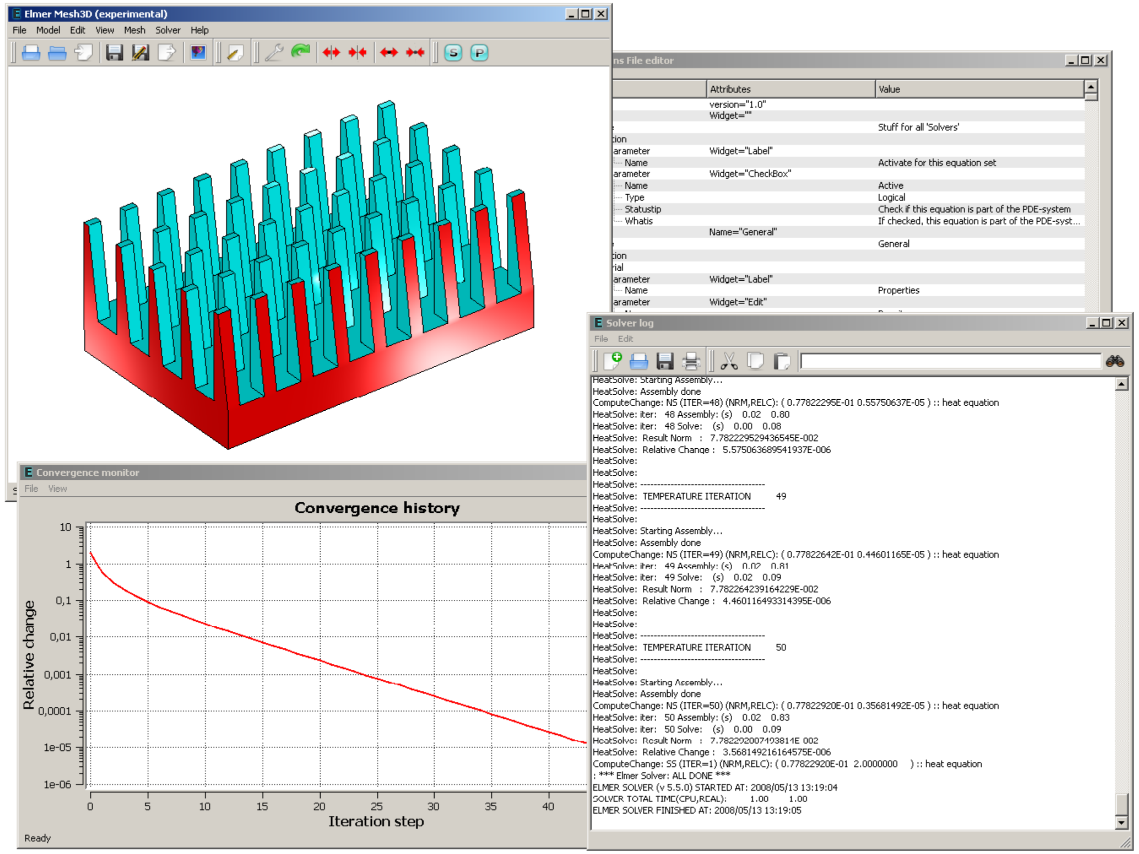
Elmer finite element software

- **Elmer** is actually a suite of several programs
  - Components may also be used independently
- **ElmerGUI** – Preprocessing
- **ElmerSolver** – FEM Solution
  - Each physical equation is a **dynamically loaded** library to the main program
- **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



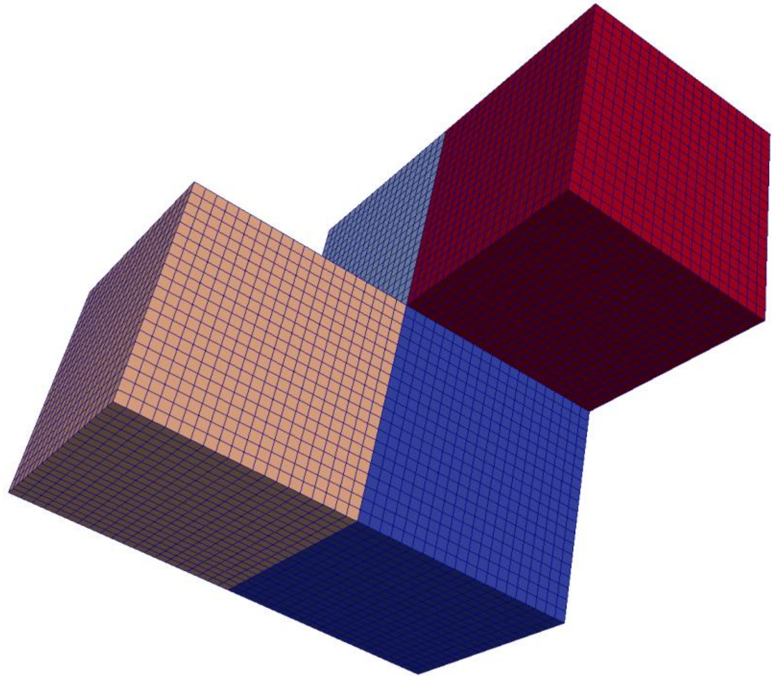
ElmerSolver

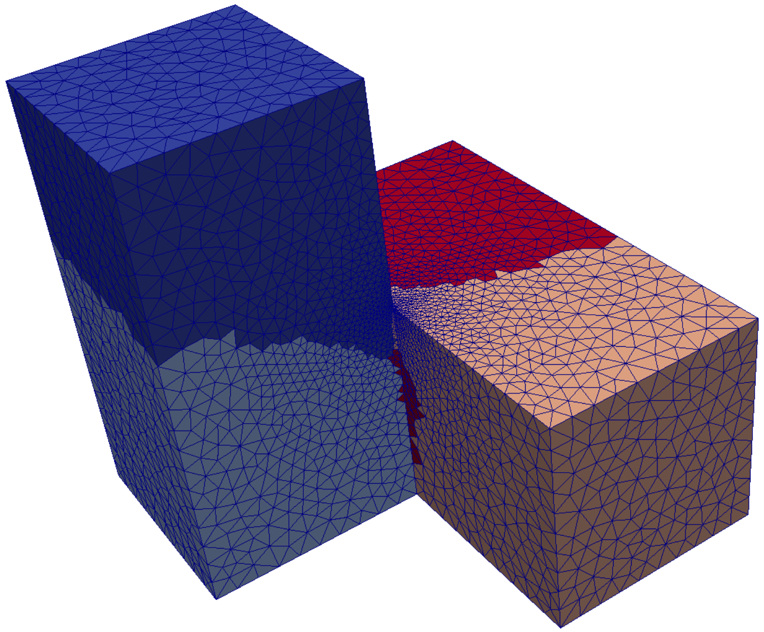
- Assembly and solution of the finite element equations and beyond
- Large number of auxiliary routines
- Note: When we talk of Elmer we mainly mean ElmerSolver
- ~95% of development effort

```
ELMER SOLVER (v 8.3) STARTED AT: 2017/06/19 18:35:01
ParCommInit:  Initialize #PEs:          1
MAIN: ==============================================================
MAIN: ElmerSolver finite element software, Welcome!
MAIN: This program is free software licensed under (L)GPL
MAIN: Copyright 1st April 1995 - , CSC - IT Center for Science Ltd.
MAIN: Webpage http://www.csc.fi/elmer, Email elmeradm@csc.fi
MAIN: Version: 8.3 (Rev: 8068c86, Compiled: 2017-06-18)
MAIN:  HYPRE library linked in.
MAIN:  MUMPS library linked in.
MAIN: ==============================================================
MAIN: Reading Model: flux.sif
LoadMesh: Base mesh name: ./angle
MAIN: -------------------------------------
Loading user function library: [HeatSolve]...[HeatSolver]
HeatSolve: -------------------------------------
HeatSolve:  TEMPERATURE ITERATION         1
HeatSolve: -------------------------------------
HeatSolve: Assembly:
DefUtils::DefaultDirichletBCs: Setting Dirichlet boundary conditions
ComputeChange: NS (ITER=1) (NRM,RELC): ( 0.25941344E-01  2.0000000     ) :: heat equation
CompareToReferenceSolution: Solver 1 PASSED:  Norm = 2.59413436E-02  RefNorm = 2.5941343
CompareToReferenceSolution: Relative Error to reference norm: 1.512027E-09
CompareToReferenceSolution: PASSED all 1 tests!
ElmerSolver: *** Elmer Solver: ALL DONE ***
ElmerSolver: The end
SOLVER TOTAL TIME(CPU,REAL):        0.10       0.15
ELMER SOLVER FINISHED AT: 2017/06/20 01:35:01
```

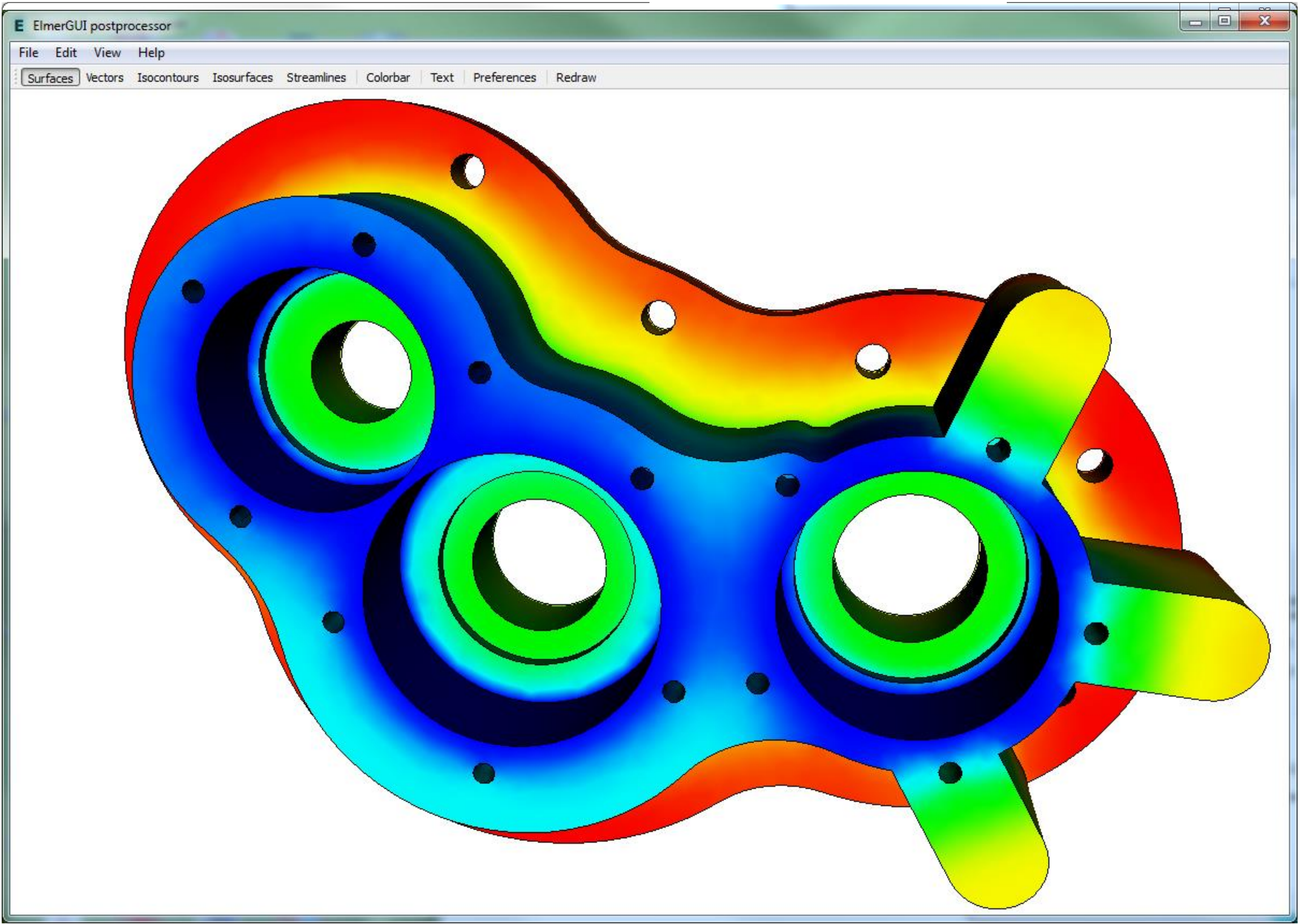
ElmerGrid (standalone + built-in ElmerGUI)

- Creation of 2D and 3D structured meshes
  - Rectangular basic topology + simple mapping
  - Extrusion, rotation
- Mesh Import
  - About ten different formats:
    Ansys, Abaqus, Fidap, Comsol, Gmsh,…
- Mesh manipulation
  - Increase/decrease order
  - Scale, rotate, translate
- Partitioning
  - Simple geometric (upper figure)
  - Metis library (lower figure)





SERIAL WORKFLOW: VISUALIZATION



$$\Omega = \bigcup \Omega_e$$

$$-\nabla \cdot \kappa \nabla T = h \ \text{ in } \Omega$$

$$T = T_0 \ \text{ at } \Gamma$$

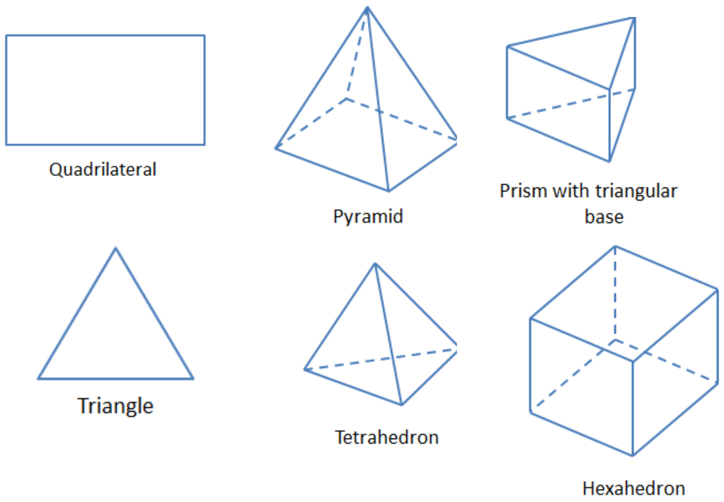
$$A_{ij} += \int \kappa \nabla \varphi_i \cdot \nabla \varphi_j \, d\Omega_e$$

$$b_i += \int h \varphi_i \, d\Omega_e$$

$$x = A^{-1} b$$

ElmerSolver – Numerical Methods

- Time-dependency
  - Static, transient, harmonic, eigenmode, scanning
- Discretization
  - Element families: nodal, edge (Hcurl), face (Hdiv), and p-elements, DG
  - Element shapes: triangles, quads, tets, wedges, pyramids, hexas
  - Formulations: Galerkin, stabilization, bubbles
  - Continuity: Mortar finite elements for periodic and nonconforming meshes

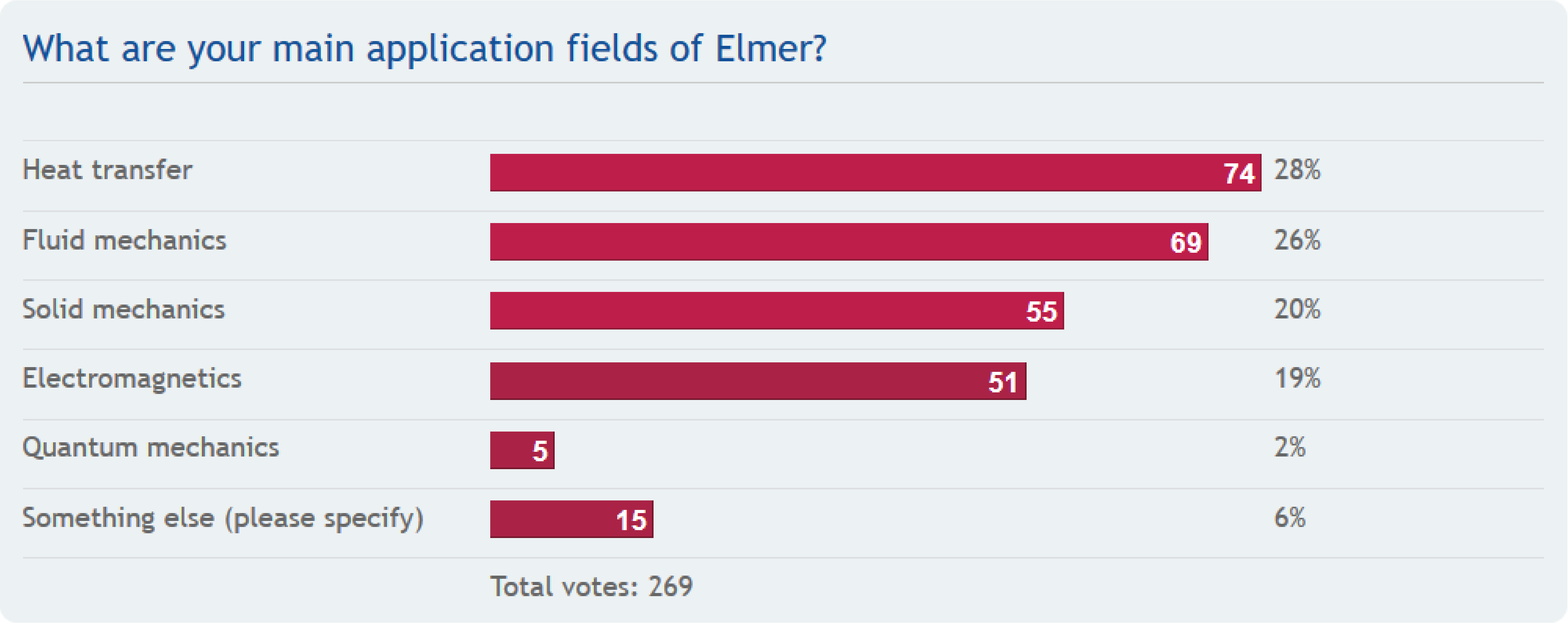


- Linear system solvers
  - Direct: Lapack, Umfpack, (SuperLU, Mumps, Pardiso)
  - Iterative Krylov space methods (HutIter & Hypre)
  - multigrid solvers (GMG & AMG) for “easy” equations (own & Hypre)
  - Preconditioners: ILU, BILU, Parasails, multigrid, SGS, Jacobi,…
- Adaptivity
  - For selected equations, unfortunately no parallel implementation

ElmerSolver - Physical Models

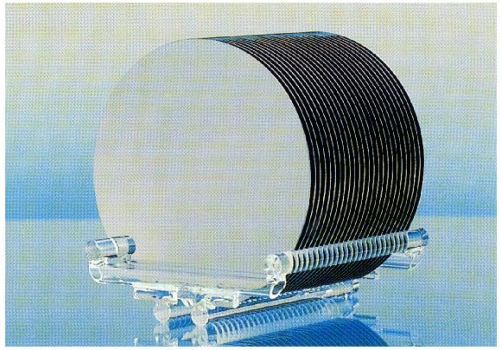
- Heat transfer
  - ✓ Heat equation
  - ✓ Radiation with view factors
  - ✓ convection and phase change
- Fluid mechanics
  - ✓ Navier-Stokes (2D & 3D)
  - ✓ RANS: *SST k-Ω, k-ε, v²-f*
  - ✓ LES: VMS
  - ✓ Thin films: Reynolds (1D & 2D)
- Structural mechanics
  - ✓ General elasticity (unisotropic, lin & 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)
  - ✓ Free surface defined by a function
- Electrokinetics
  - ✓ Poisson-Boltzmann
- Thermoelectricity
- Quantum mechanics
  - ✓ DFT (Kohn Scham)
- Particle Tracker

Poll on application fields (status 3/2020)

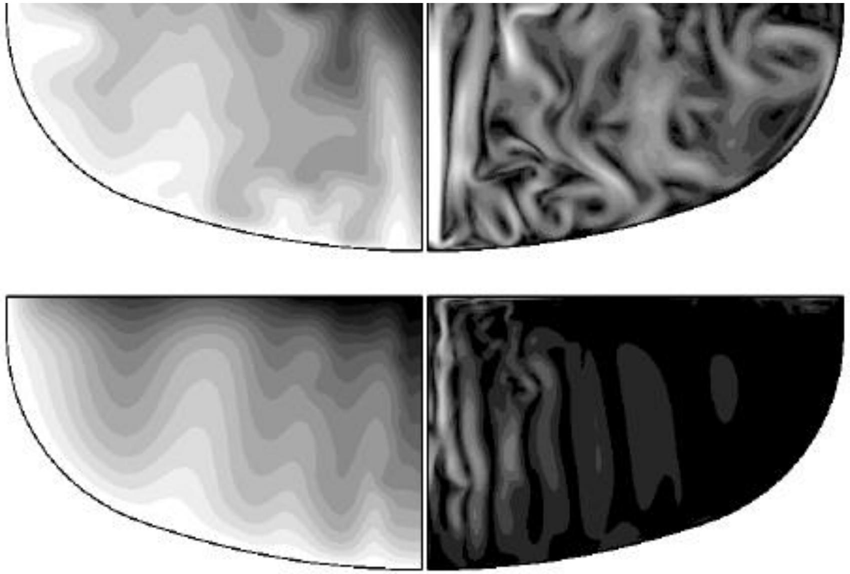


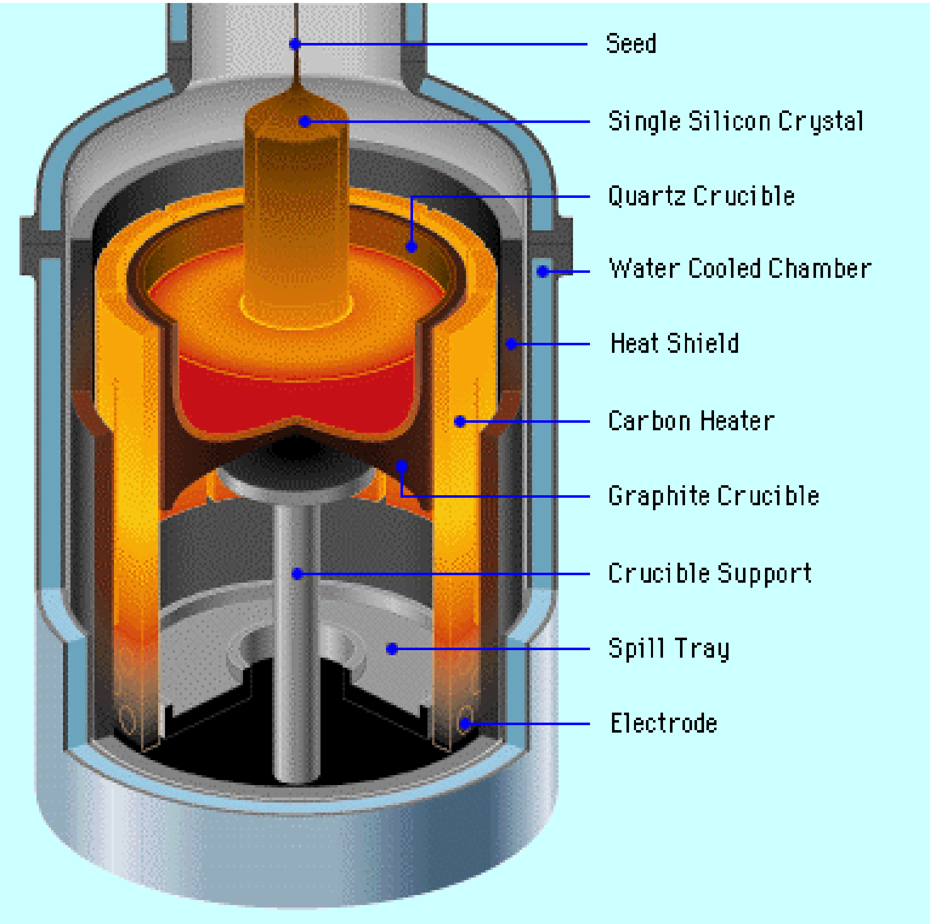
Czockralski Crystal Growth

- Most crystalline silicon is grown by the Czhockralski (CZ) method
- The main application when Elmer development was started.



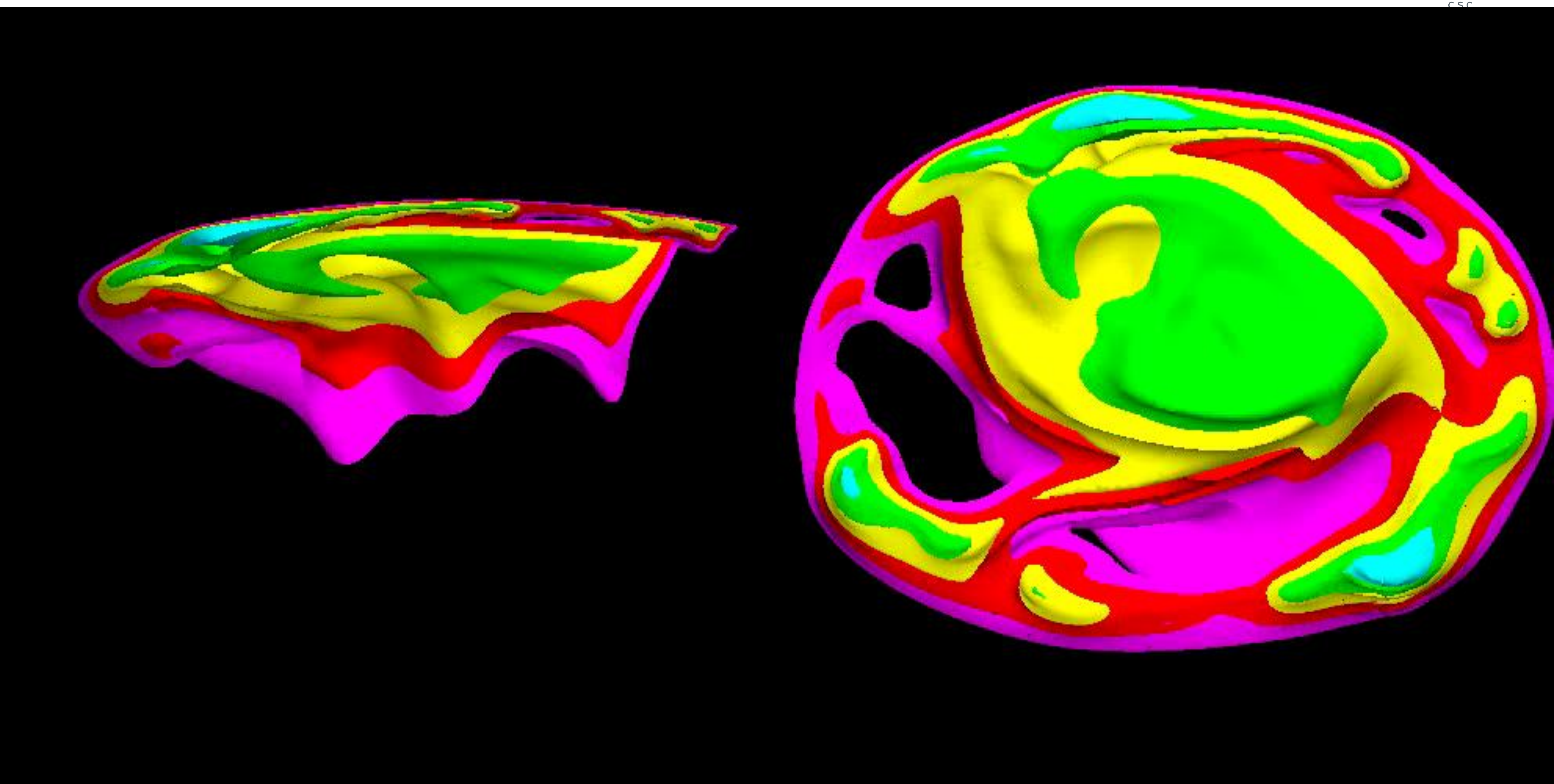
Figures by Okmetic Ltd.



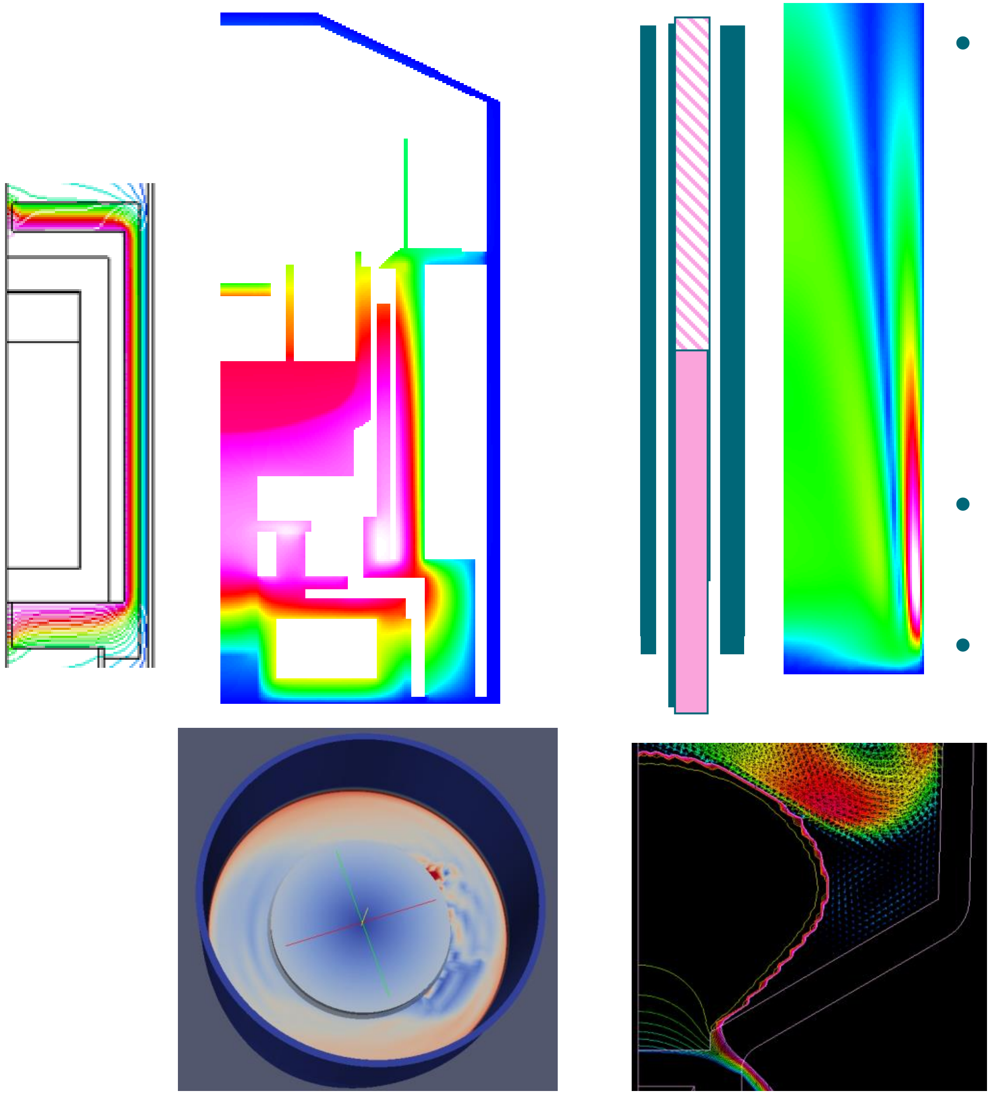


V. Savolainen et al., *Simulation of large-scale silicon melt flow in magnetic Czochralski growth*, J. Crystal Growth 243 (2002), 243-260.

CZ-growth: Transient simulation



Elmer in Crystal Growth Simulations



- Elmer has been used extensively in crystal growth simulations: These include crystal and tube growth for silicon, silicon-carbide, NiMnGa and sapphire in Czochralski, HTCVD, sublimation, Bridgman, Vertical Gradient Freeze and Heat Exchanger Methods.
- Numerical results have been successfully verified with experiments.
- Elmer is a part of open-source chain from CAD to visualization, and offers an access to parallelism and a number of simultaneous simulations important for industrial R&D.

Simulations Jari Järvinen, Silicom Oy, 2014

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

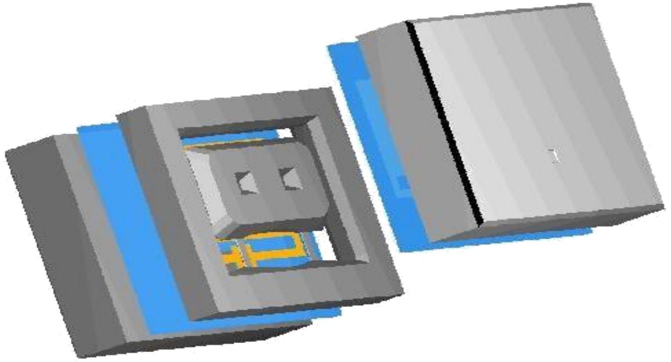
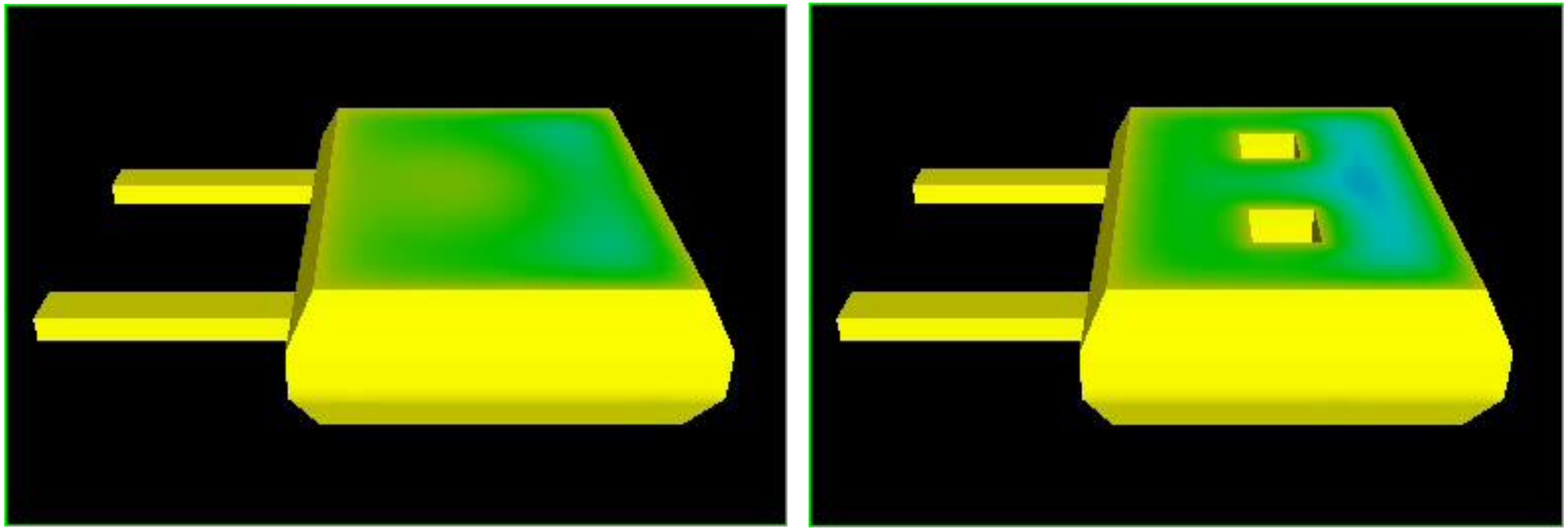


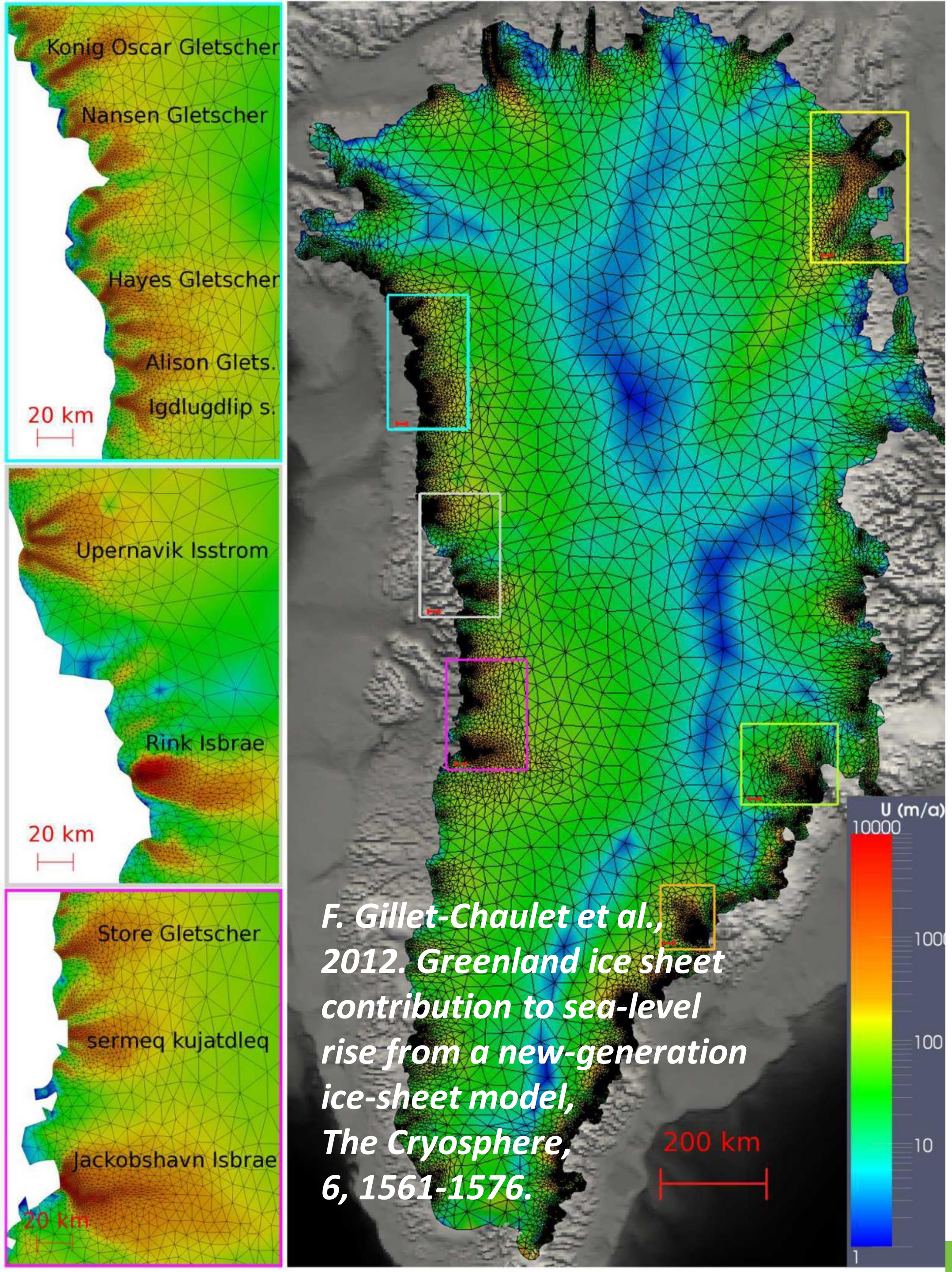
Figure by VTI Technologies



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.

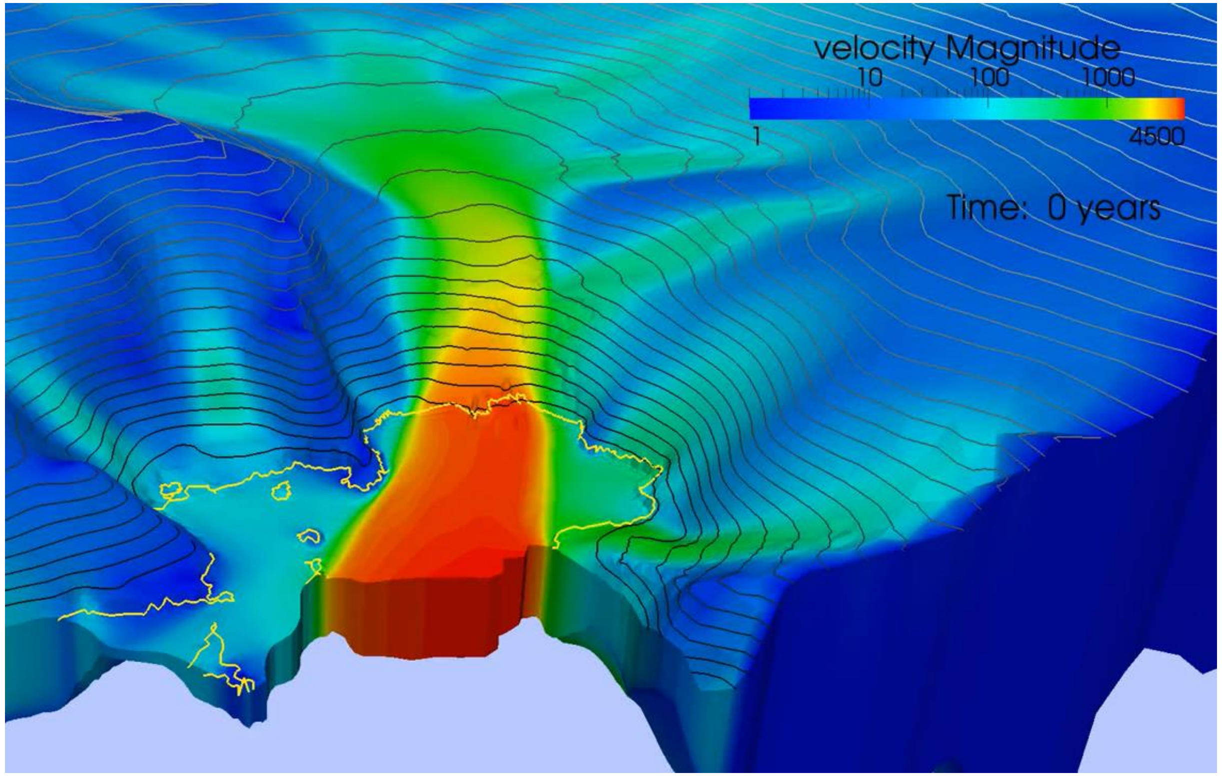
Elmer/ICE: Glaceology

- **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
- Currently ~100 peer-reviewed publications in the area
- Dedicated community portal `elmerice.elmerfem.org`



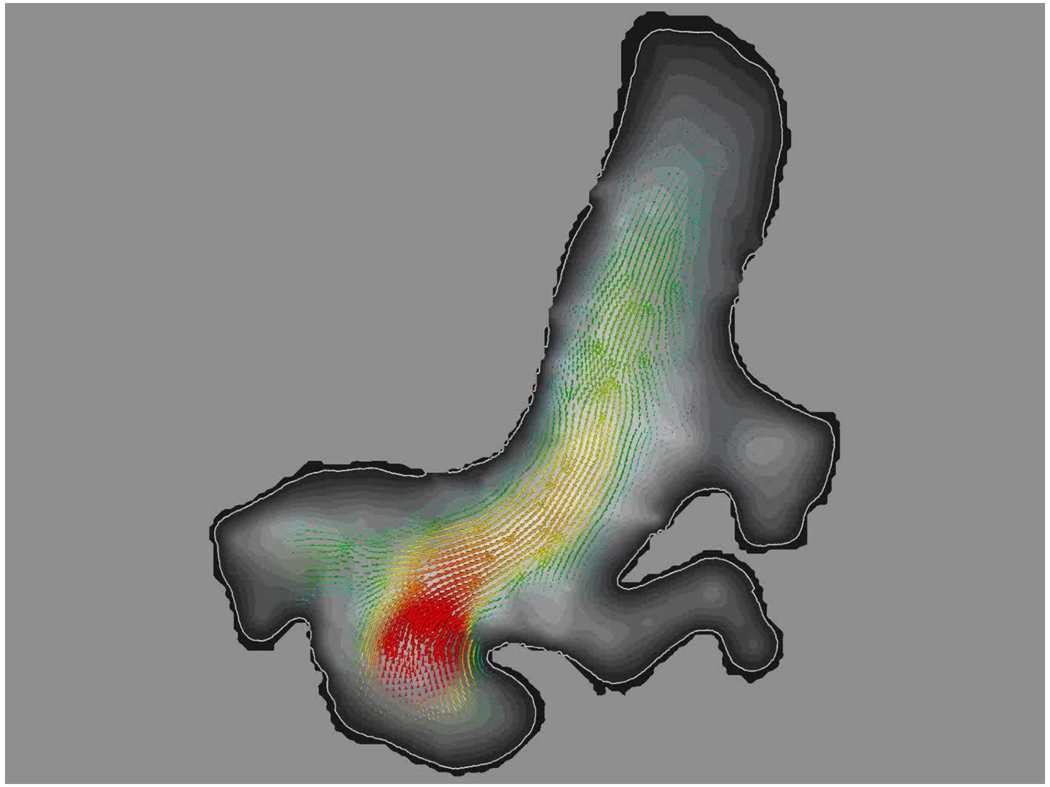
F. Gillet-Chaulet et al., 2012. Greenland ice sheet contribution to sea-level rise from a new-generation ice-sheet model, The Cryosphere, 6, 1561-1576.

Marine Ice Sheets



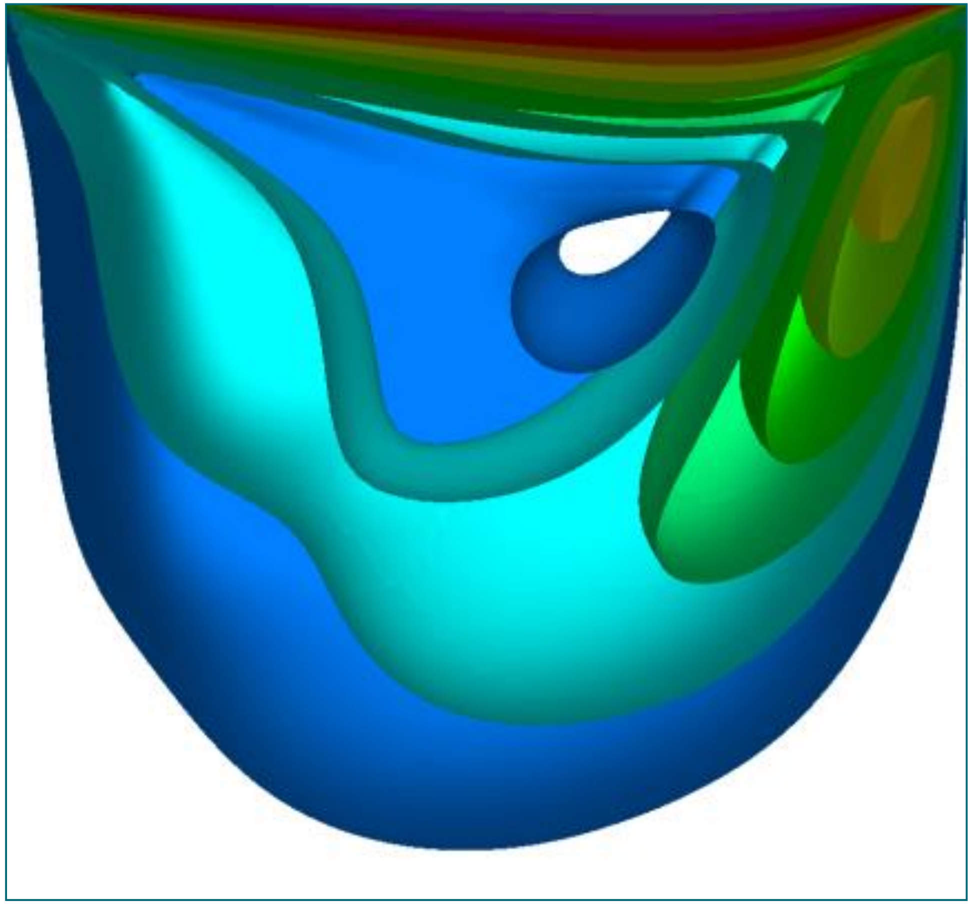
Favier, L., G. Durand, S. L. Cornford, G. H. Gudmundsson, O. Gagliardini, F. Giller-Chaulet, T. Zwinger, A. J. Payne and A. M. Le Brocq, 2014. ***Retreat of Pine Island Glacier controlled by marine ice-sheet instability***, Nature Climate Change

Glaciers



T. Zwinger and Moore, J. C. (2009) ***Diagnostic and prognostic simulations with a full Stokes model accounting for superimposed ice of Midtre Lovénbreen****, Svalbard*, The Cryosphere, 3, 217-229, doi:10.5194/tc-3-217-2009

Block preconditioning: Weak scaling of 3D driven-cavity



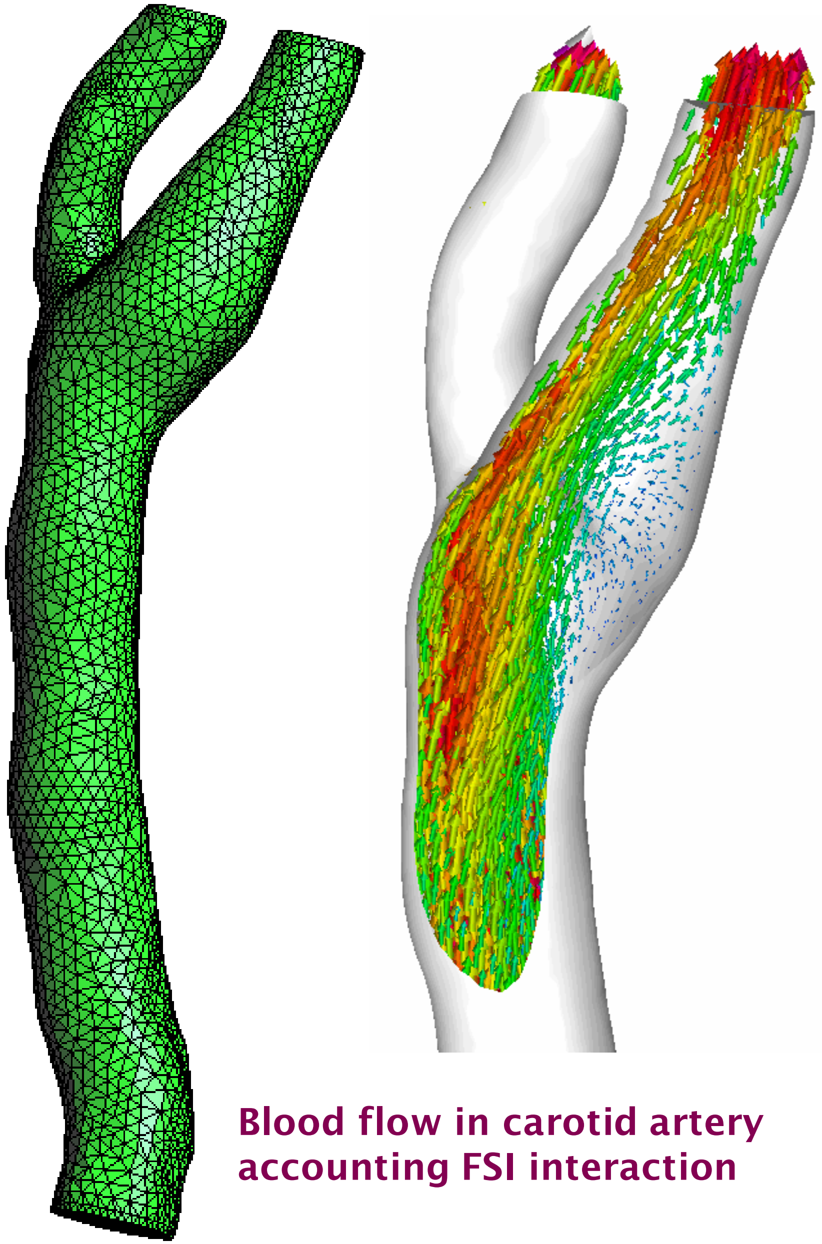
Elems	Dofs	#procs	Time (s)
34^3	171,500	16	44.2
43^3	340,736	32	60.3
54^3	665,500	64	66.7
68^3	1,314,036	128	73.6
86^3	2,634,012	256	83.5
108^3	5,180,116	512	102.0
132^3	9,410,548	1024	106.8

Velocity solves with Hypre: CG + BoomerAMG preconditioner for the 3D driven-cavity case (Re=100) on Cray XC (Sisu).
Simulation Mika Malinen, CSC.

O(~1.14)

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

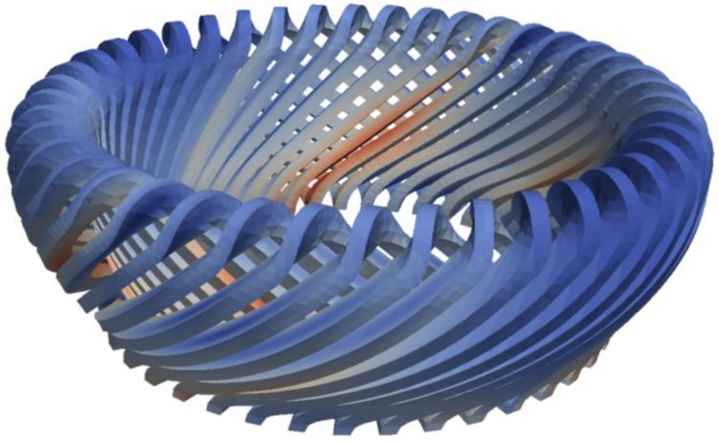


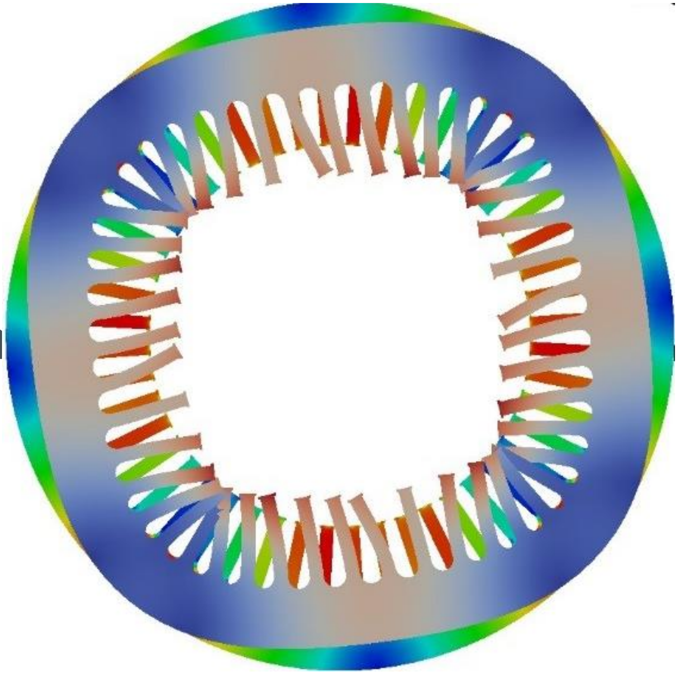
Blood flow in carotid artery accounting FSI interaction

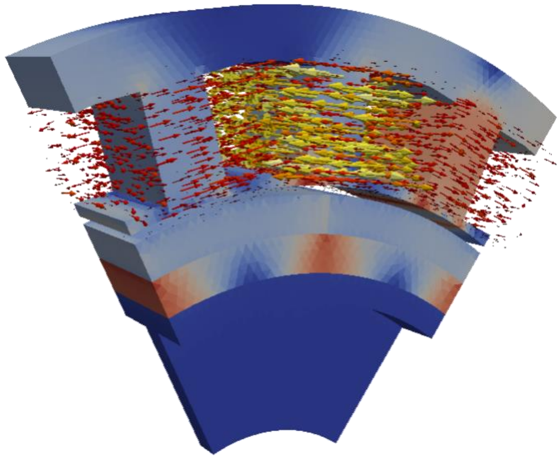
E. Järvinen, P. Råback, M. Lyly, J. Salonius. *A method for partitioned fluid-structure interaction computation of flow in arteries. Medical Eng. & Physics*, **30** (2008), 917-923

Elmer/EM: Collaboration in electromechanics

- SEMTEC project to further develop Elmer as a tool for heavy electromagnetics computations.
  - Existing solution provided unsatisfactory scalability
  - CSC, VTT, Aalto Univ., TUT, LUT, ABB, Kone, Konecranes, Sulzer, Ingersoll-Rand, Trafotek, Scanveir
- With the end of the project large developments made available under open source
- Most important industrial application area at the moment

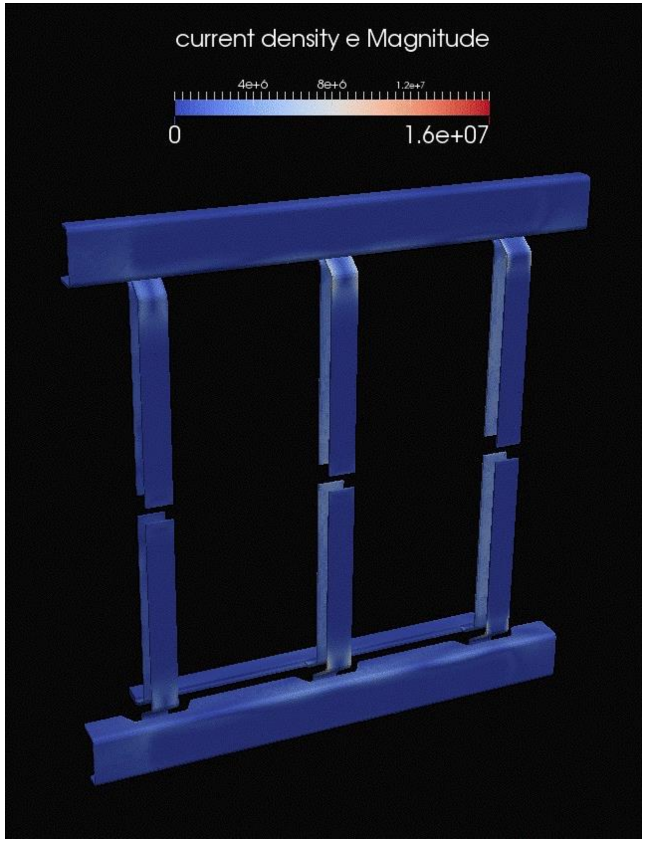


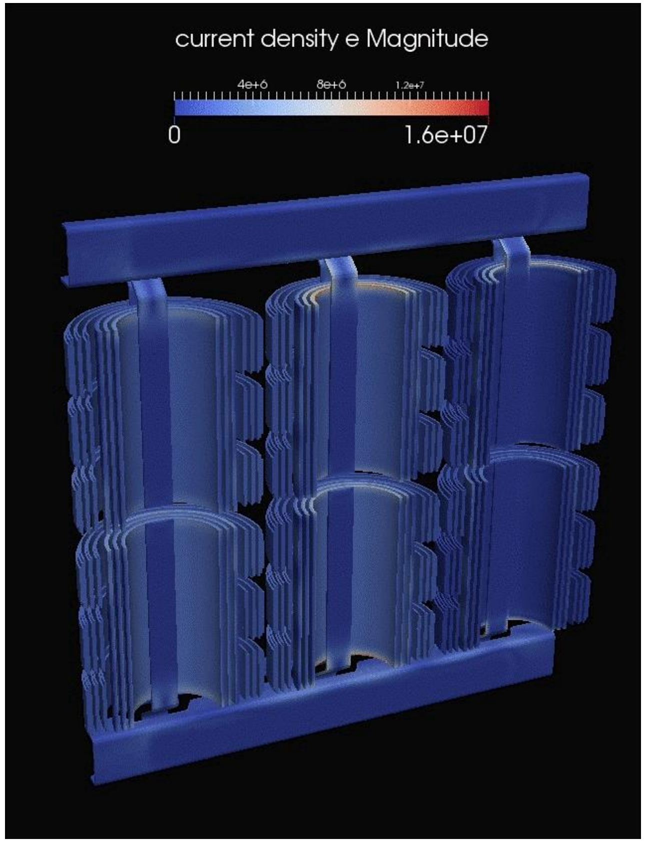




Open source workflow at Trafotek

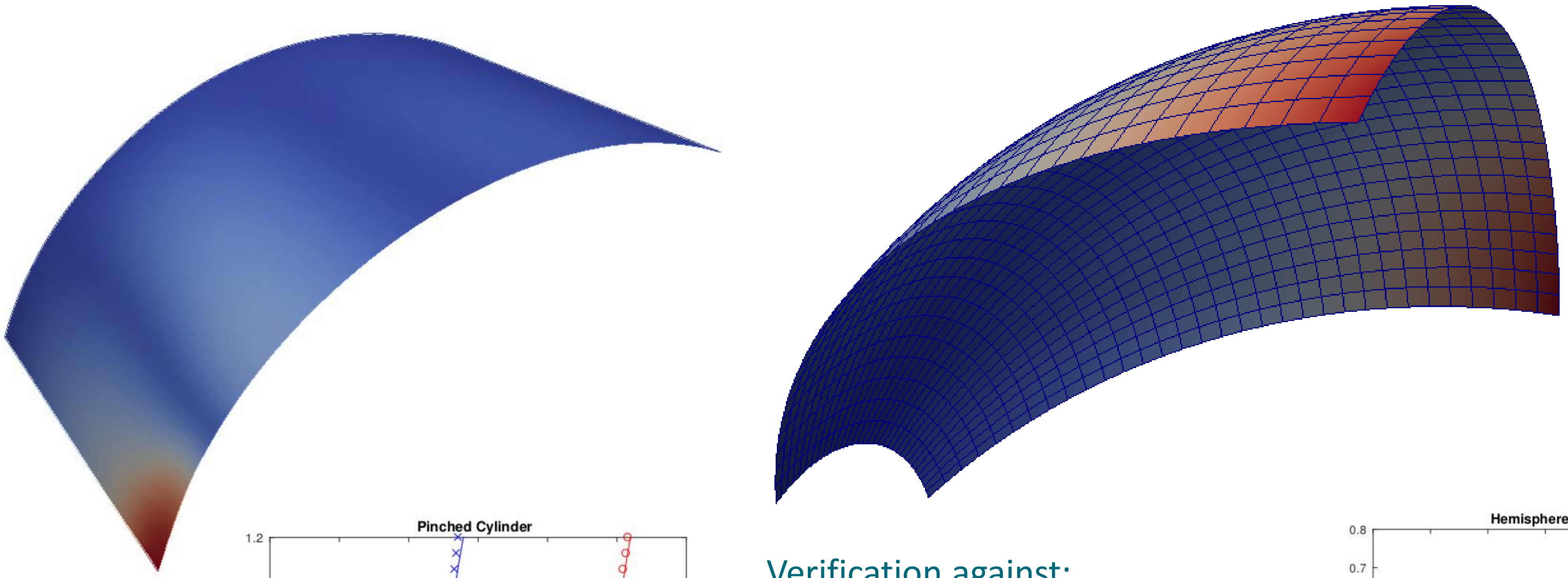
- Simulation of losses in Cast Resin Transformer by Trafotek
    - Computed with 256 cores
- CAD & meshing with **SALOME** using python bindings
- Simulation with **Elmer**
    - Estimation of heat generation from magnetic losses
    - Coupled heat and N-S equations
- Postprocessing with **Paraview**

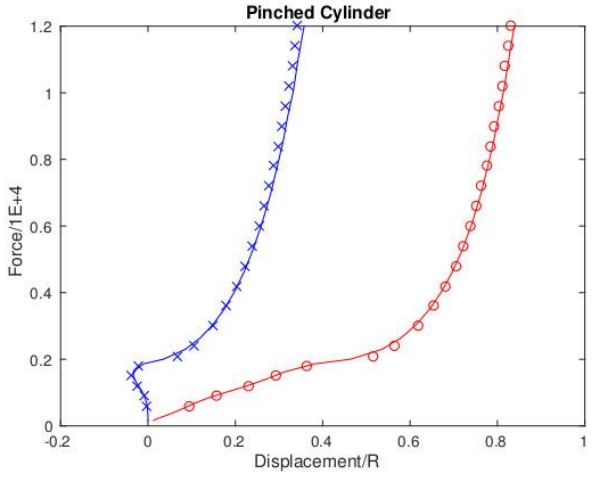




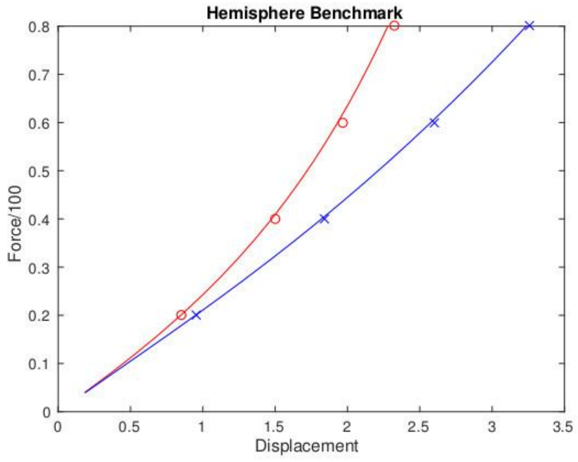
Simulation by Eelis Takala, Trafotek, Finland, 2014

Recent developments: nonlinear shell solver

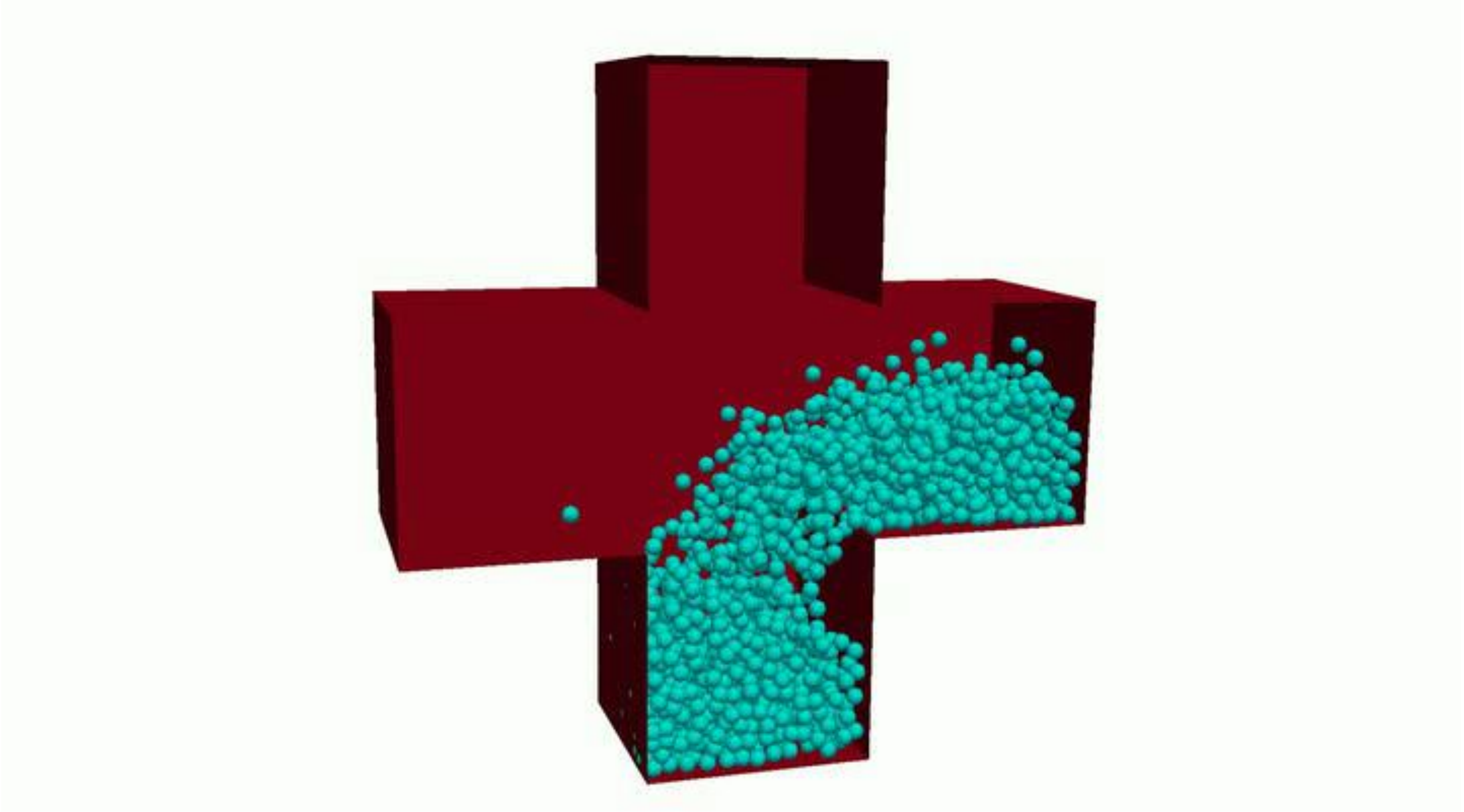




Verification against:
Sze KY, Liu XH, Lo SH, *Popular benchmark problems for geometric nonlinear analysis of shells*, Finite Elements in Analysis and Design 2004, **40**(11):1551-1569.



Elastic particles - Granular flow



Simulation Peter Råback, CSC, 2011.

pyelmer

- The pyelmer package provides a simple object-oriented way to set up Elmer simulations from python.
- Some utility-functions for pre-processing using the gmsh python API, execution of ElmerGrid and ElmerSolver, and some post-processing routines are provided. Some default simulation settings, solvers, and materials are available.
- GitHub: https://github.com/nemocrys/pyelmer
- Pypi: https://pypi.org/project/pyelmer/

LATVIJAS UNIVERSITATE
ANNO 1919

EOF-Library

Video
& info

Elmer and **OpenFOAM** coupler

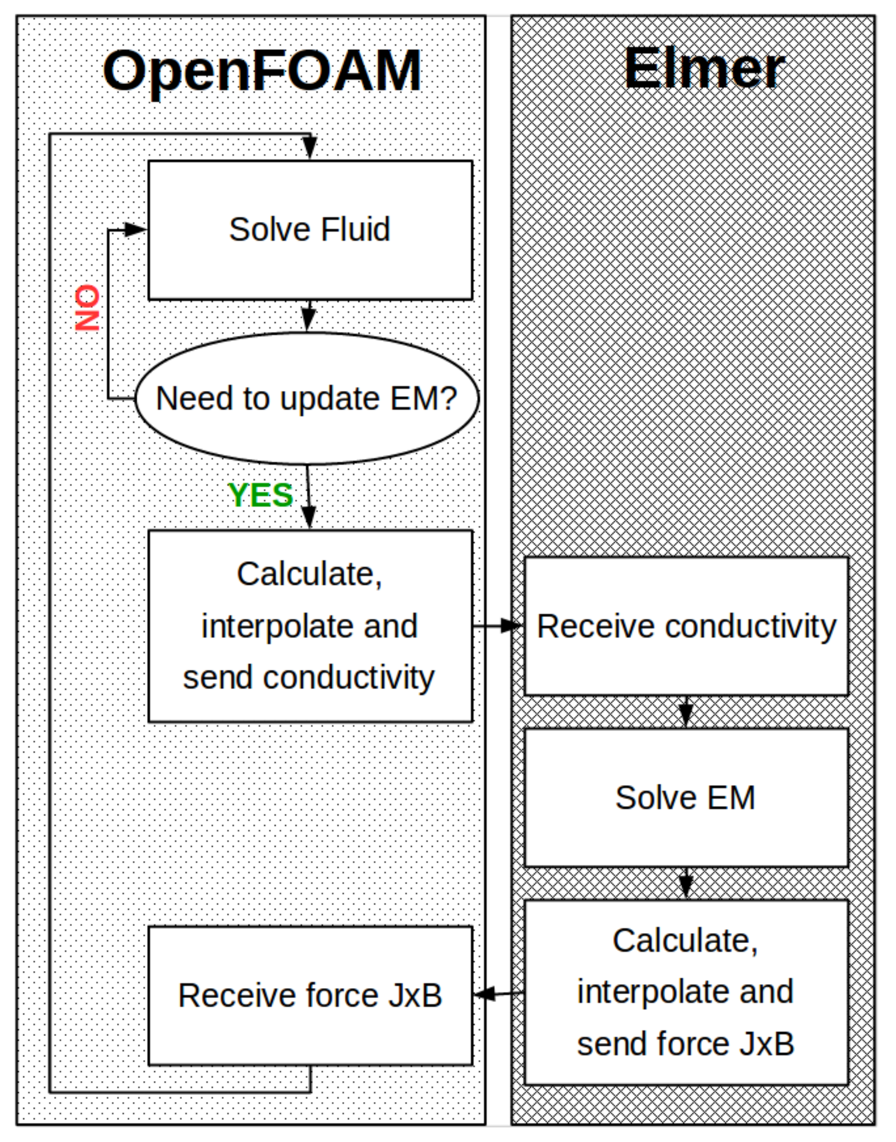
- Open-source
- MPI-based
- 4 dynamic libraries + solvers

Multiphysics coupling

- Electromagnetics
- Fluids with free surface
- Heat transfer

Running both codes simultaneously

mpirun -n x Elmer : -n y OpenFOAM



Concluding remarks about Elmer

- Developed mainly via collaborative projects with academia and industry
  - MEMS, Microfluidics, Acoustics, Crystal Growth, Hemodynamics, Glaciology, Electromagnetics,…
- Focus on developments where open source approach is natural
  - Science: Compatibe with the scientific method
  - Novel developments: benefit from the fast feedback cycle of open source software
- Little emphasis on the GUI
  - Serious users mainly use Elmer in scripted workflows
  - Complementary rather than competing to commercial codes
- Value stability and backward compability – consistency tests
- Favour modularity and generality for multiphysics
- Always consider parallellism and scalability

Most important Elmer resources

- http://www.csc.fi/elmer
  - Official Homepage of Elmer
- http://www.elmerfem.org
  - Discussion forum, wiki, elmerice community
- https://github.com/elmercsc/elmerfem
  - GIT version control (the future)
- http://youtube.com/elmerfem
  - Youtube channel for Elmer animations
- http://www.nic.funet.fi/pub/sci/physics/elmer/
  - Download repository
- Further information: peter.raback@csc.fi

Thank you for your attention!