Elmer

Open Source Finite Element Software for Multiphysical Problems

ElmerTeam
CSC – IT Center for Science

Elmer course
CSC, 1.-2.6.2017

What is CSC?

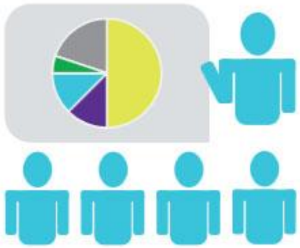
- Founded in 1971 as a technical support unit for Univac 1108
- Connected Finland to the Internet in 1988
- Owned by the the Universities and Ministry of Education and Culture of Finland
- Offers IT resources for **research**, education, culture and administration
- Operates on a **non-profit** principle
- Facilities in Espoo, close to Otaniemi campus and Kajaani
- Staff ~300
- Currently official name is: ”**CSC – IT Center for Science”**

CSC's Services

Scientific Computing and Software

Funet Network Services

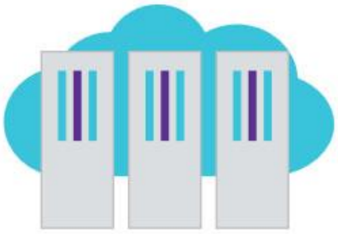
Identity and Access Management



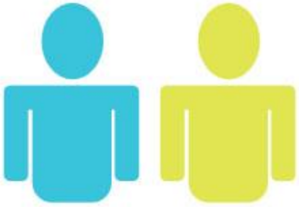
Training services

Research Information Management

Education Management and Student Administration Services

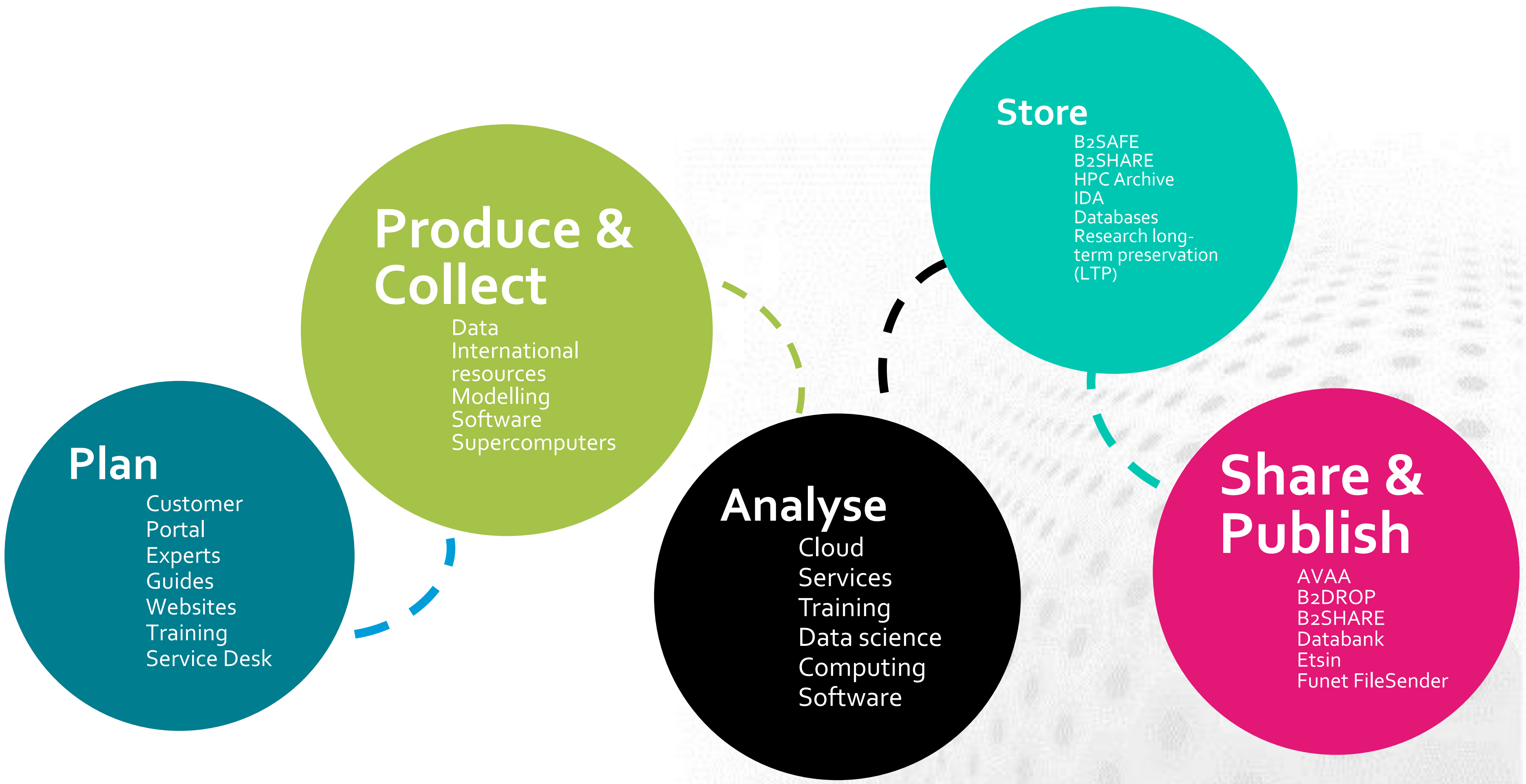


Datacenter and Capacity Services



Consultation and Tailored Solutions

Support in All Phases of Research Process

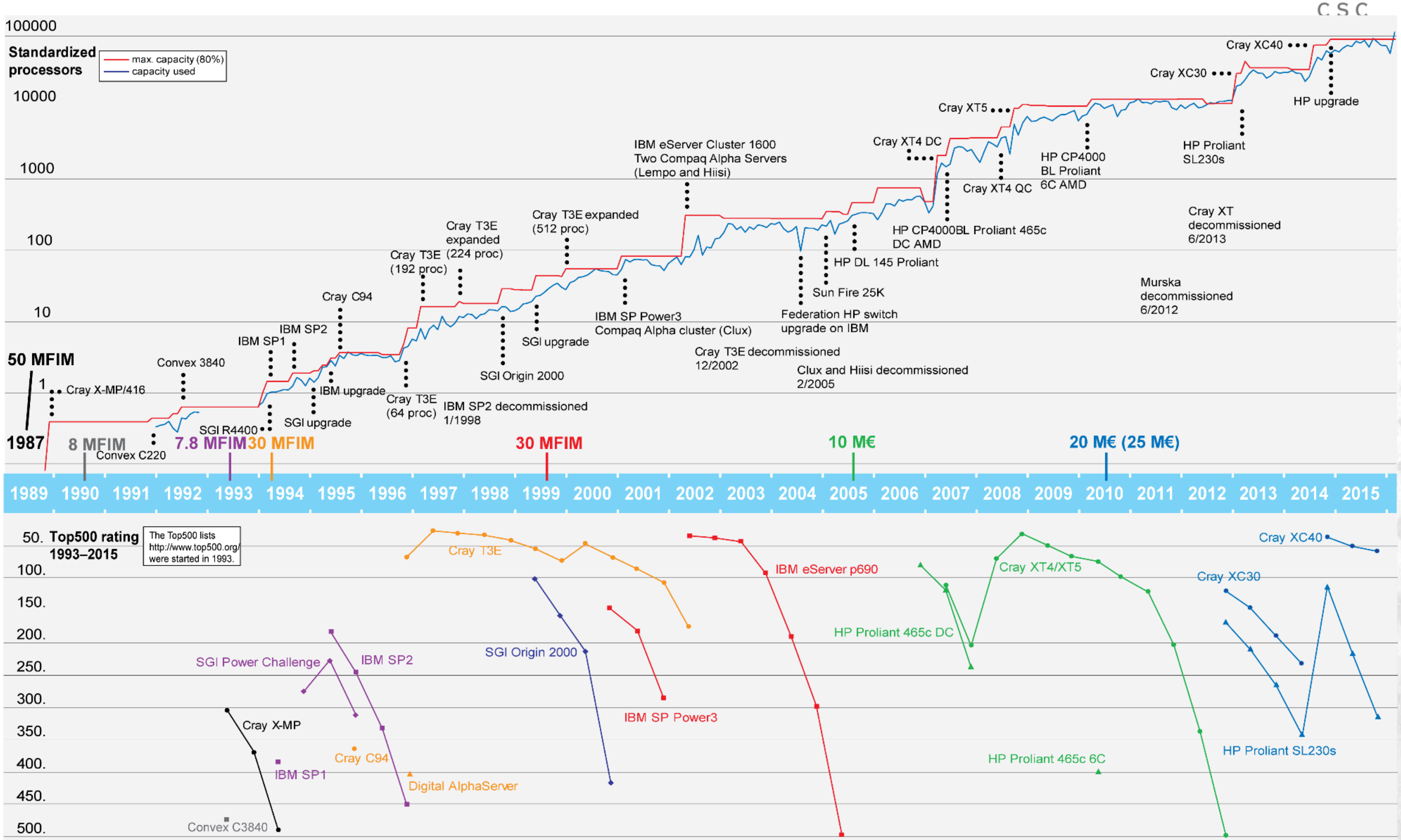


CSC's Computing Services

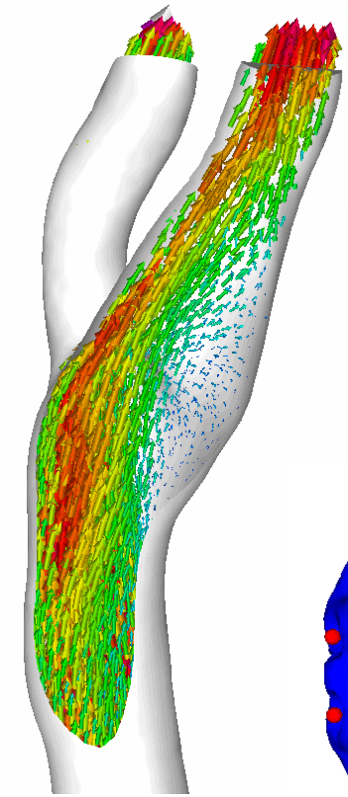
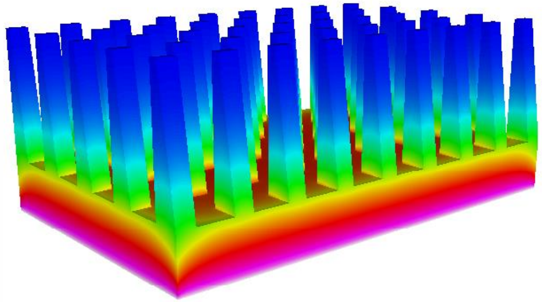
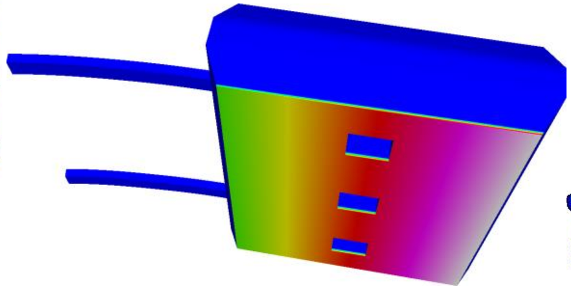
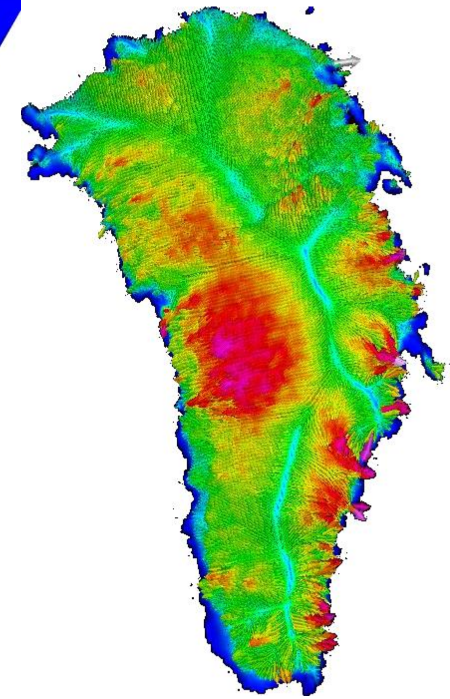
Performance	Capacity	Special processors	Cloud	Hosting
Sisu	Taito	Bull/Taito extension	cPouta	Kajaani Espoo
40 512 cores	18 816 cores	996 cores	Cores provisioned from Taito cluster	
Aries interconnect	InfiniBand interconnect	76 Nvidia K40 GPUs 90 Intel Xeon Phi 7120X		
>4PB, ~ 100GB/s				

Storage services

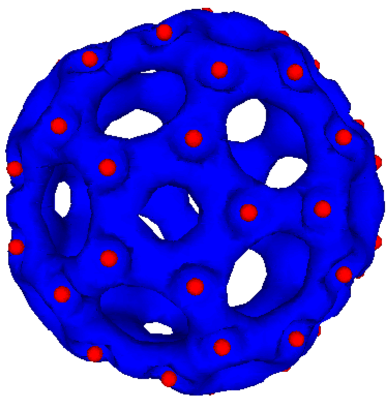
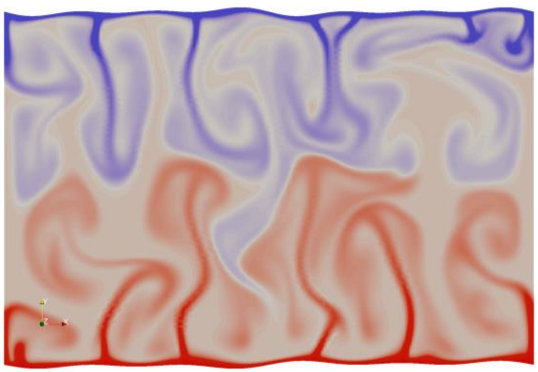
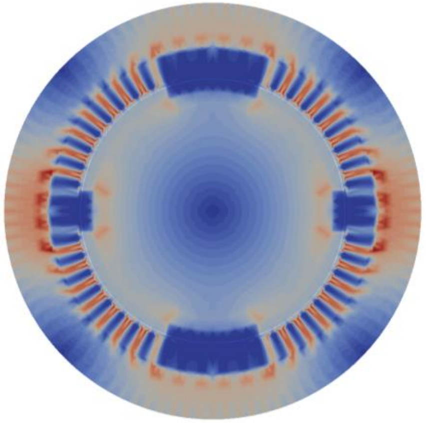
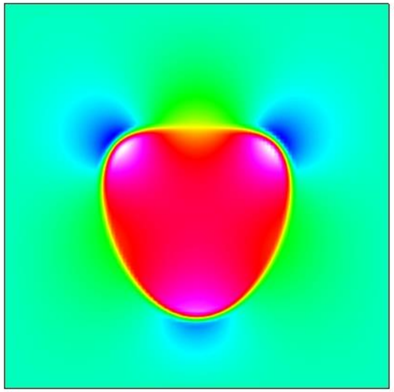
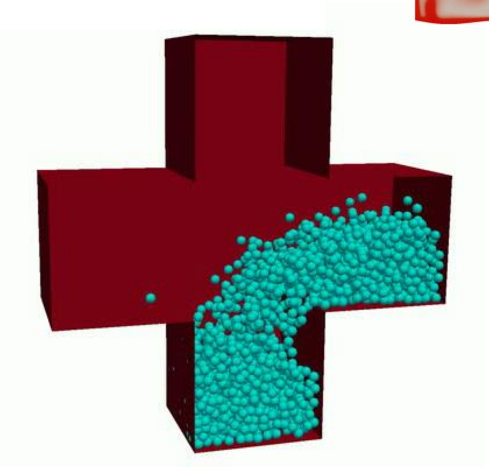
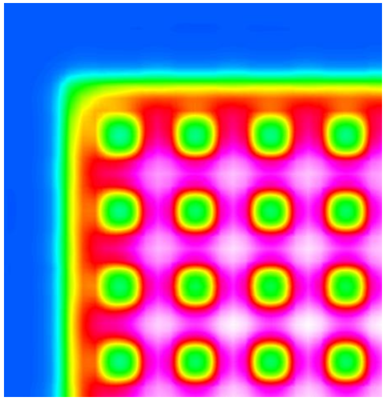
CSC's Computing Capacity 1989–2015



In 2015: About 2700 active users

Elmer finite element software for multiphysical problems

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

Some Pros and Cons of Finite Element Method

- Applicable to **arbitrary shapes**
  - #1 method in engineering
- Non-uniform mesh refinement
- Based on variational principle
  - Approaches functional to be minimized from above
  - **Monotonic convergence** with mesh size parameter
- Suited for all kinds of PDEs
  - Elliptic, hyperbolic, parabolic
- Natural treatment of BCs
- Vast mathematical literature supports the method

- For problems without ”shape” and uniform meshes the additional cost of FEM may not be well motivated
  - Indirect memory addressing of sparse matrices
- More complex machinery may take focus from the real problem
  - Mesh generation, involved mathemetatics, bigger codes, more complex data structures etc.

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, Electromagnetics,…
- 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, Juhani Kataja
- Other/past developers & contributors
  - CSC: Mikko Lyly, Mikko Byckling, Sampo Sillanpää, Jussi Heikonen, Esko Järvinen, Jari Järvinen, Antti Pursula, Ville Savolainen, Sami Ilvonen, Erik Edelmann
  - VTT: Pavel Ponomarev, Janne Keränen, Paul Klinge, Martti Verho
  - TKK: Jouni Malinen, Harri Hakula, Mika Juntunen
  - Trafotek: Eelis Takala
  - LGGE: Olivier Gagliardini, Fabien Gillet-Chaulet,…
  - University of Uppsala: Jonas Thies, Josefin Ahlkrona
  - etc… (if your name is missing, please ask it to be added)

Elmer in numbers (11/2015)

Software

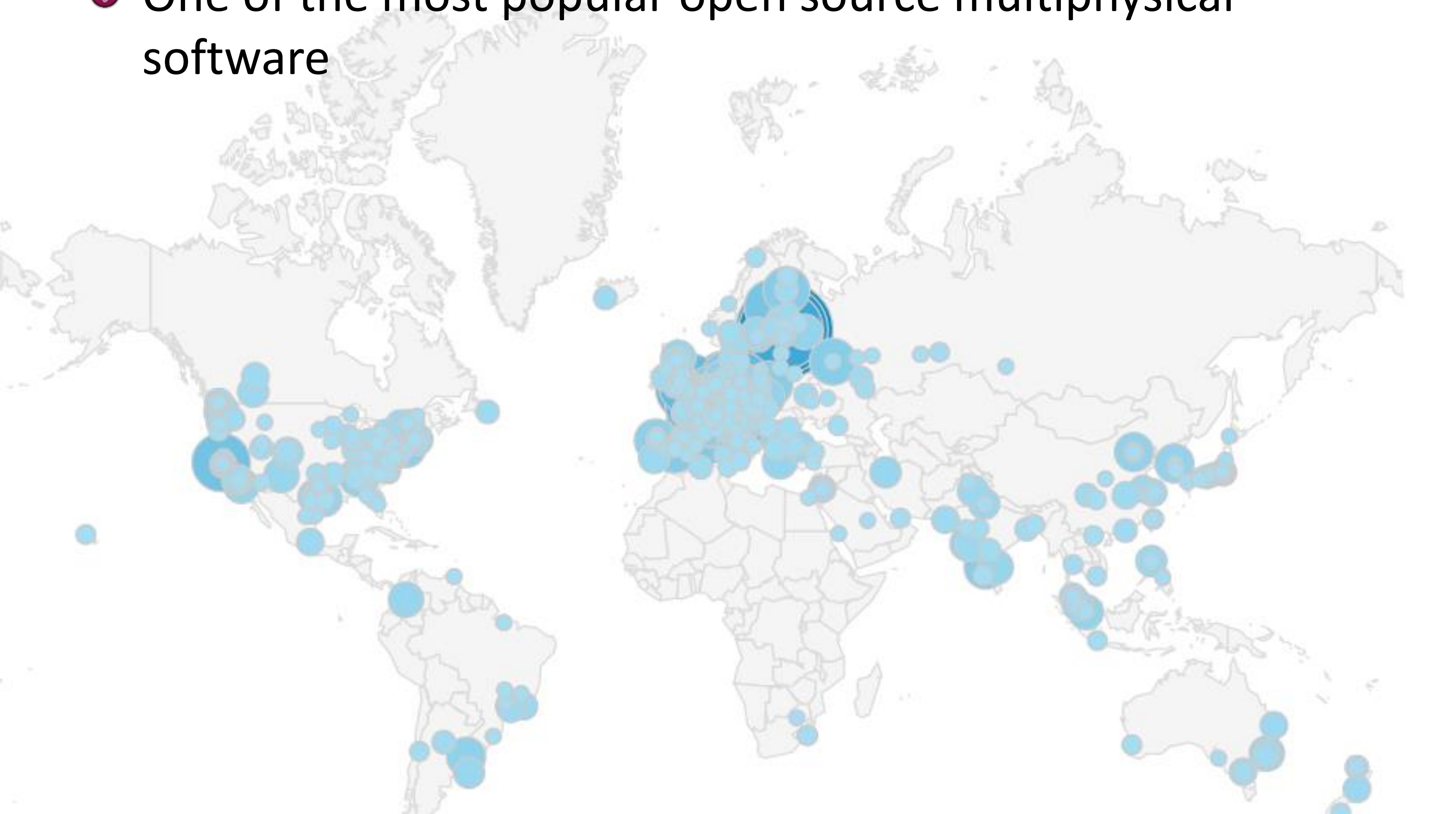
- ~400,000 lines of active code
  - ~3/4 in Fortran, 1/4 in C/C++
- ~540 consistency tests
- ~750 pages of documentation
- ~1000 code commits yearly

Community

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

Elmer is published under (L)GPL

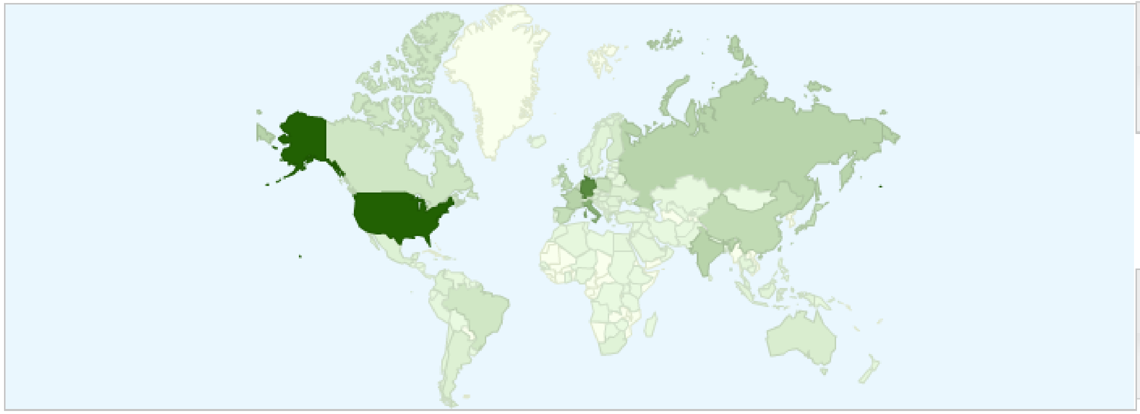
- Used worldwide by thousands of researchers (?)
- One of the most popular open source multiphysical software



~20k Windows downloads at sf.net in a year

Home / WindowsBinaries (Change File)

Date Range: 2012-04-01 to 2013-03-31



DOWNLOADS
19 185
In the selected date range

TOP COUNTRY
United States
16% of downloaders

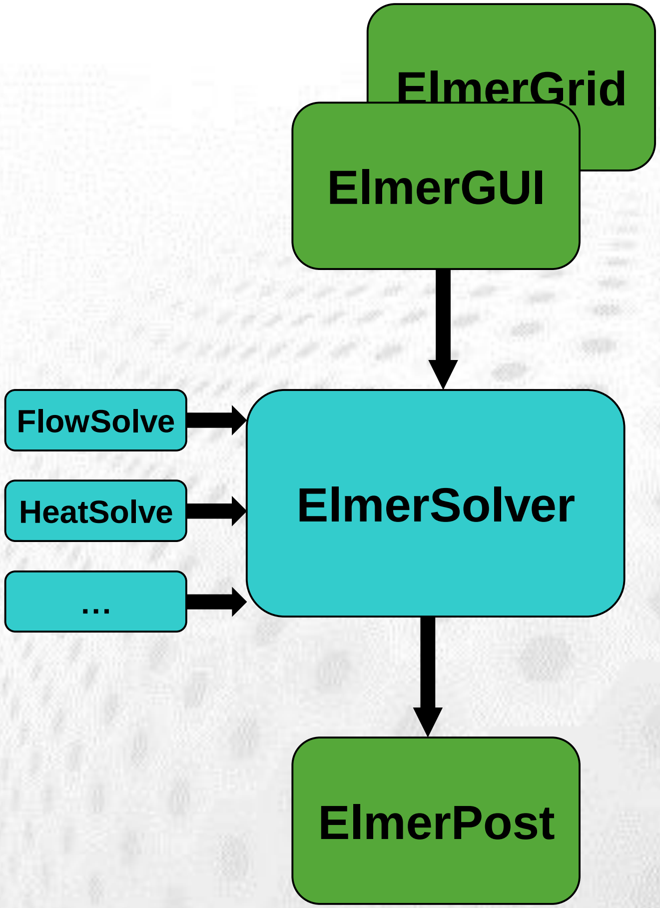
TOP OS
Windows
93% of downloaders

OS downloads as: Percent

	Country	Android	BSD	Linux	Macintosh	Unknown	Windows	Total
1.	United States	0%	0%	3%	3%	1%	80%	3,182
2.	Germany	0%	0%	4%	1%	0%	80%	2,313
3.	Italy	0%	0%	3%	1%	0%	80%	1,537
4.	France	0%	0%	4%	1%	1%	79%	798
5.	India	0%	0%	6%	1%	4%	78%	782
6.	Russia	0%	0%	4%	0%	0%	77%	772
7.	United Kingdom	0%	0%	3%	2%	0%	81%	642
8.	China	0%	0%	3%	1%	1%	78%	637
9.	Japan	0%	0%	2%	2%	0%	77%	599
10.	Spain	0%	0%	6%	0%	20%	63%	561
11.	Poland	0%	0%	2%	0%	0%	87%	532
12.	Canada	1%	0%	2%	2%	0%	85%	410
13.	Brazil	0%	0%	4%	1%	0%	88%	391
14.	Finland	0%	0%	2%	1%	0%	78%	300

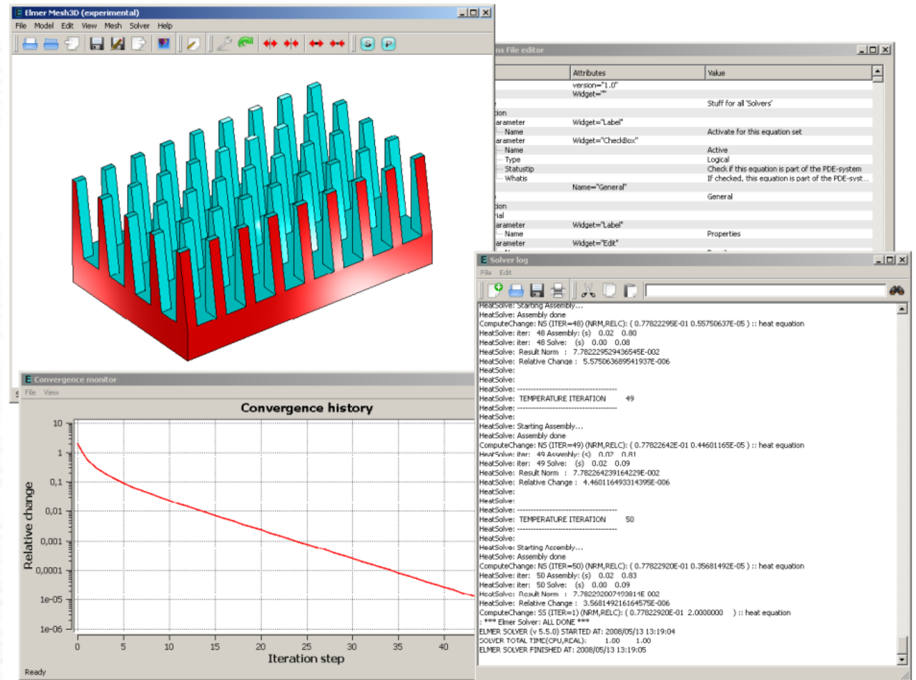
Elmer finite element software

- **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
- **ElmerGrid** – structured meshing, mesh import & partitioning
- **ElmerPost** - Postprocessing



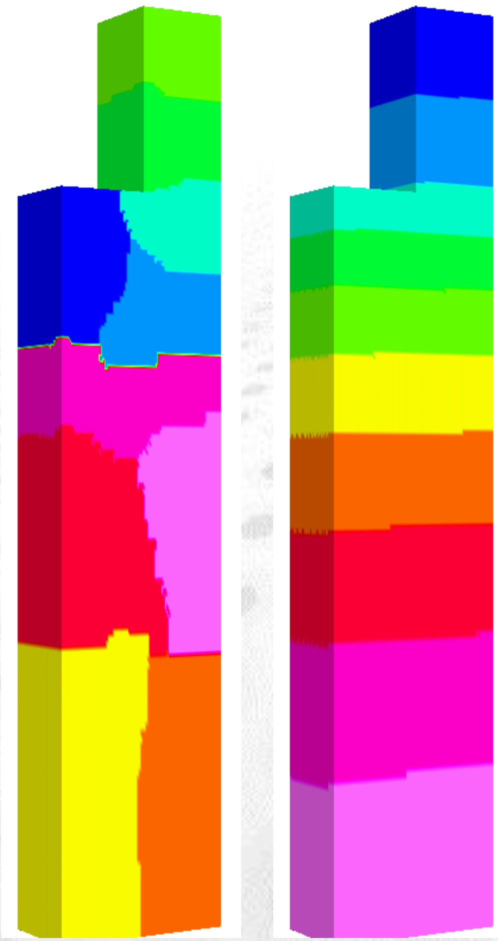
ElmerGUI

- 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 built-in postprocessing with **ElmerVTK**



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,…
  - Gmsh import example:
    >ElmerGrid 14 2 mesh.msh -autoclean
- Mesh manipulation
  - Increase/decrease order
  - Scale, rotate, translate
- Partitioning
  - Simple geometry based partitioning
  - Metis partitioning example:
    >ElmerGrid 1 2 step.grd -metis 10
- Usable via ElmerGUI
  - All features not accessible (e.g. partitioning)

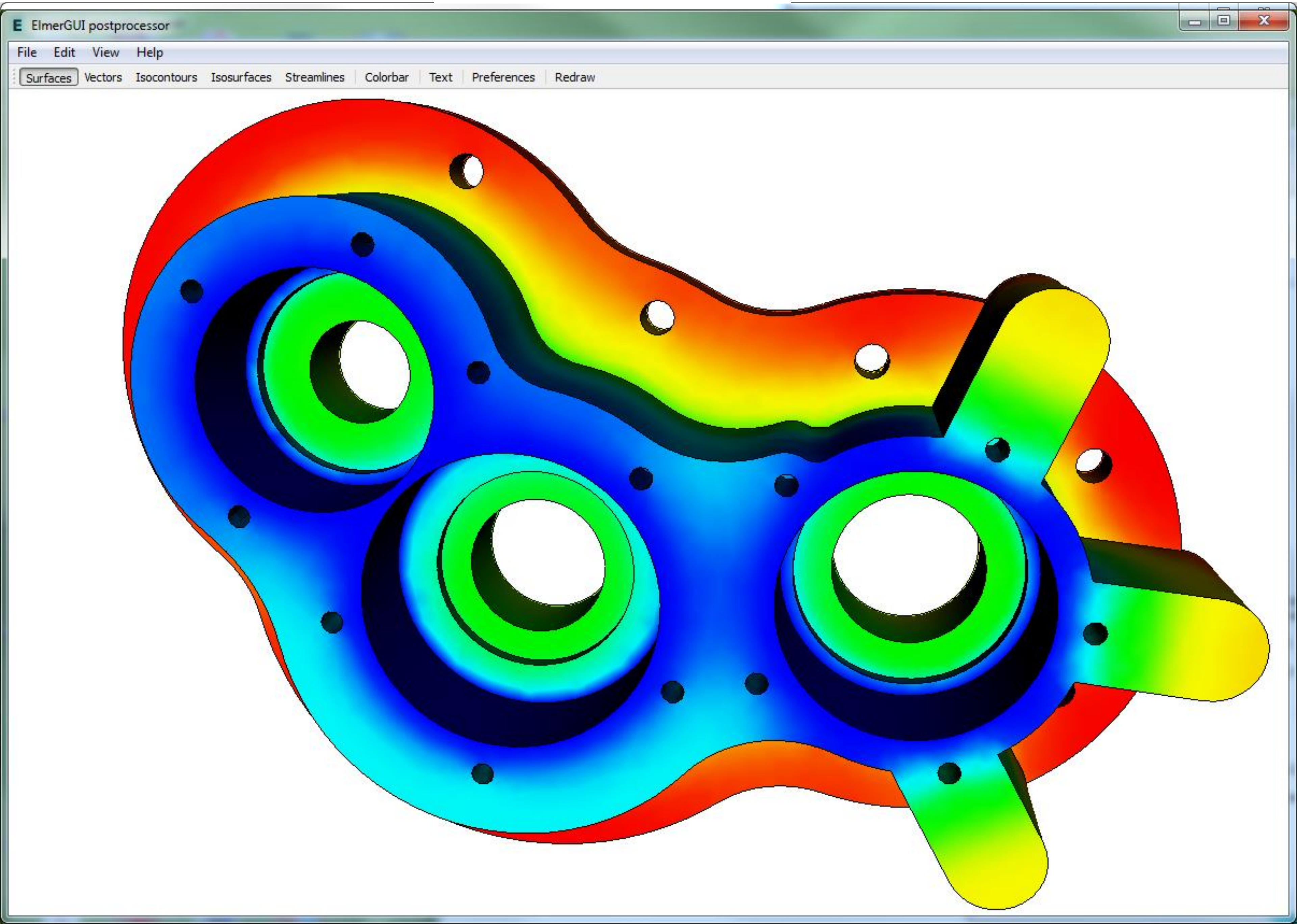


ElmerSolver

- 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

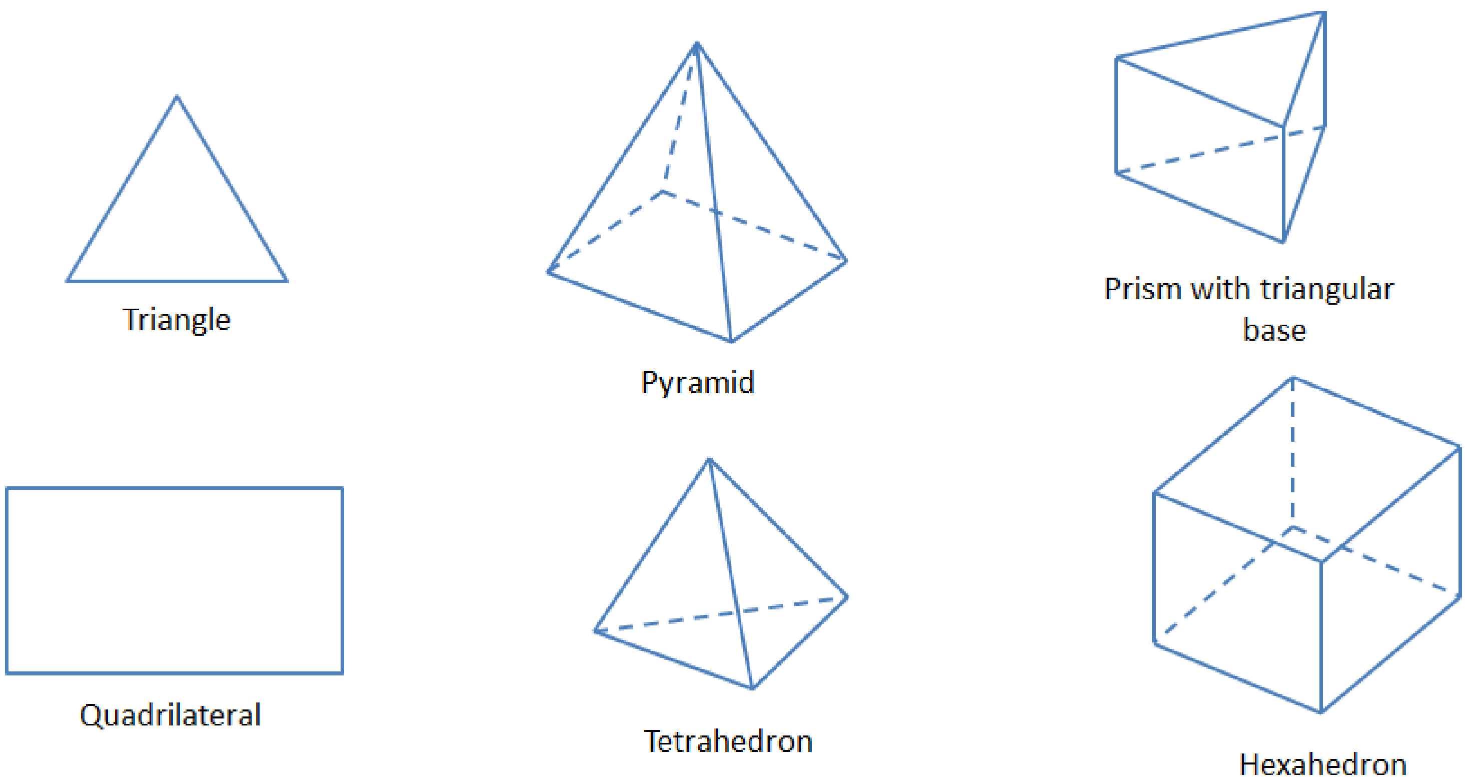
```
raback@hippu4:/fs/elmer/elmerfem/fem/tests/heateq> ElmerSolver
ELMER SOLVER (v 7.0) STARTED AT: 2014/10/15 18:44:51
MAIN:
MAIN: =============================================================
MAIN: ElmerSolver finite element software, Welcome!
MAIN: This program is free software licensed under (L)GPL
MAIN: Copyright 1st April 1995 - , CSC - IT Center for Science Ltd.
MAIN: Webpage http://www.csc.fi/elmer, Email elmeradm@csc.fi
MAIN: Library version: 7.0 (Rev: 6927M)
MAIN: =============================================================
MAIN:
MAIN: -------------------------------------
MAIN: Reading Model: TempDist.sif
...
HeatSolve: -------------------------------------
HeatSolve:  TEMPERATURE ITERATION         1
HeatSolve: -------------------------------------
HeatSolve:
HeatSolve: Starting Assembly...
HeatSolve: Assembly done
ComputeChange: NS (ITER=1) (NRM,RELC): ( 0.76801649E-01  2.0000000     ) :: he1
...
HeatSolve: -------------------------------------
HeatSolve:  TEMPERATURE ITERATION        10
HeatSolve: -------------------------------------
HeatSolve:
HeatSolve: Starting Assembly...
HeatSolve: Assembly done
ComputeChange: NS (ITER=10) (NRM,RELC): ( 0.76801649E-02 0.10526316     ) :: he1
...
ElmerSolver: *** Elmer Solver: ALL DONE ***
ElmerSolver: The end
SOLVER TOTAL TIME(CPU,REAL):        1.09        1.18
ELMER SOLVER FINISHED AT: 2014/10/15 18:44:52
```

SERIAL WORKFLOW: VISUALIZATION



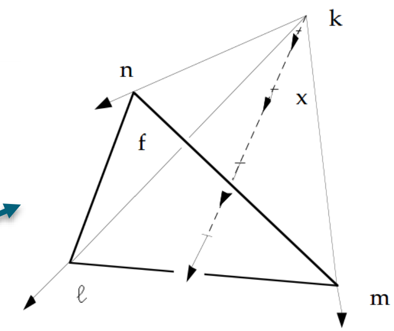
ElmerSolver – Finite element shapes

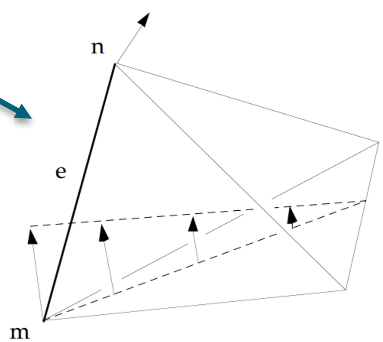
- 0D: vertex
- 1D: edge
- 2D: triangles, quadrilateral
- 3D: tetrahedrons, prisms, pyramids, hexahedrons



ElmerSolver – Finite element basis functions

- Element families
  - Nodal (up to 2-4th degree)
  - p-elements (up to 10th degree)
  - 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





Mapping & Projectors

- For conforming and nonconforming meshes
- For boundary and bulk meshes
- On-the-fly interpolation (no matrix created)
  - Mapping of finite element data
    - from mesh to mesh
    - From boundary to boundary
  - Mapping of data between particles and finite elements
    - Finite element fields at particle locations
    - Particle data to nodal field values
- Creation of interpolation and projection matrices
  - Strong continuity, interpolation: $x_l = P x_r$
  - Weak continuity, Mortar projector: $Q x_l - P x_r = 0$

ElmerSolver – Time dependency modes

- Steady-state simulation
- Transient simulation
  - 1st 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
- 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
- Direct solvers
  - Lapack (banded), Umfpack
  - Optional: SuperLU, MUMPS, Pardiso

Application examples of Elmer

Poll on application fields (status 5/2017)

What are your main application fields of Elmer?

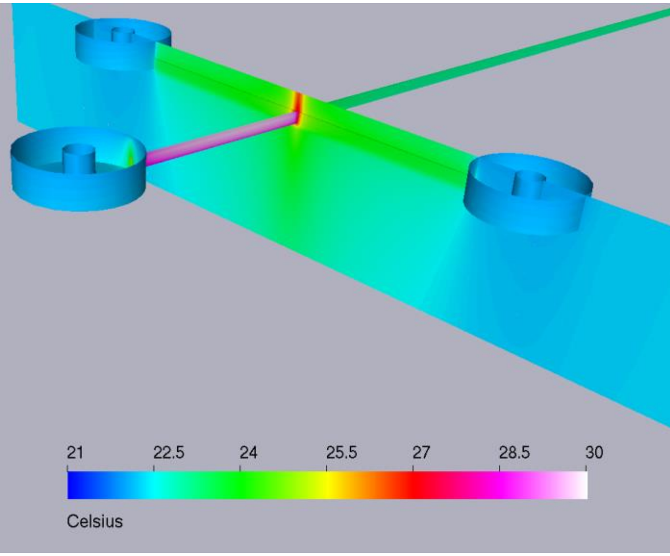
Heat transfer	70	28%
Fluid mechanics	65	26%
Solid mechanics	50	20%
Electromagnetics	43	17%
Quantum mechanics	4	2%
Something else (please specify)	14	6%
	Total votes : 246	

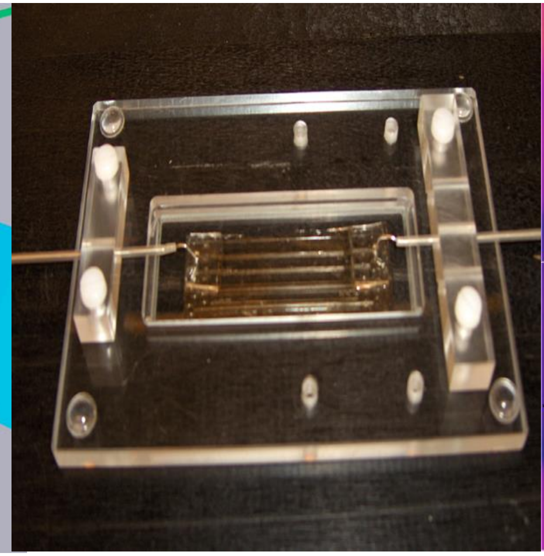
Elmer – Heat Transfer

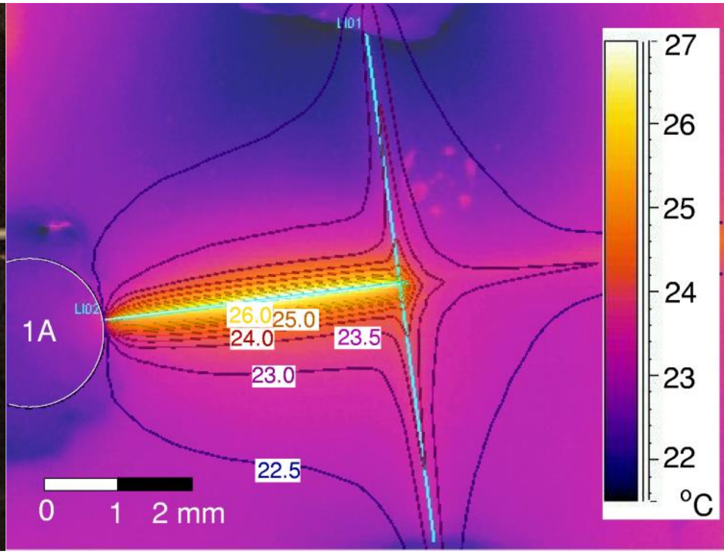
- Heat equation
  - convection
  - diffusion
  - Phase change
  - Temperature control feedback
  - Thermal slip BCs for small Kn number
- Radiation with view factors
  - 2D, axisymmetric use numerical integration
  - 3D based on ray tracing
  - Stand-alone program
- Strongly coupled thermoelectric equation

- 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

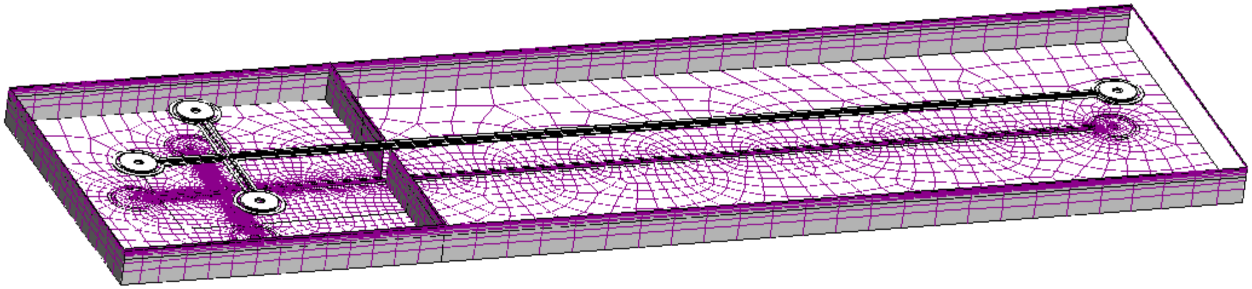
Microfluidics: Flow and heat transfer in a microchip







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



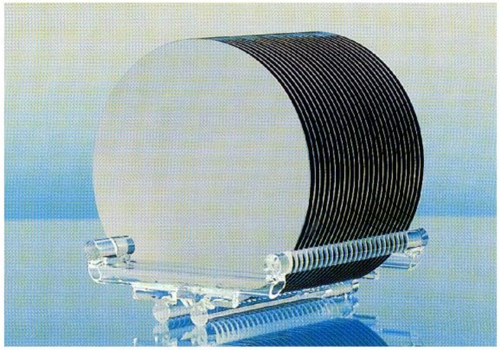
T. Sikanen, T. Zwinger, S. Tuomikoski, S. Franssila, R. Lehtiniemi, C.-M. Fager, T. Kotiaho and A. Pursula, Microfluidics and Nanofluidics (2008)

Elmer – Fluid Mechanics

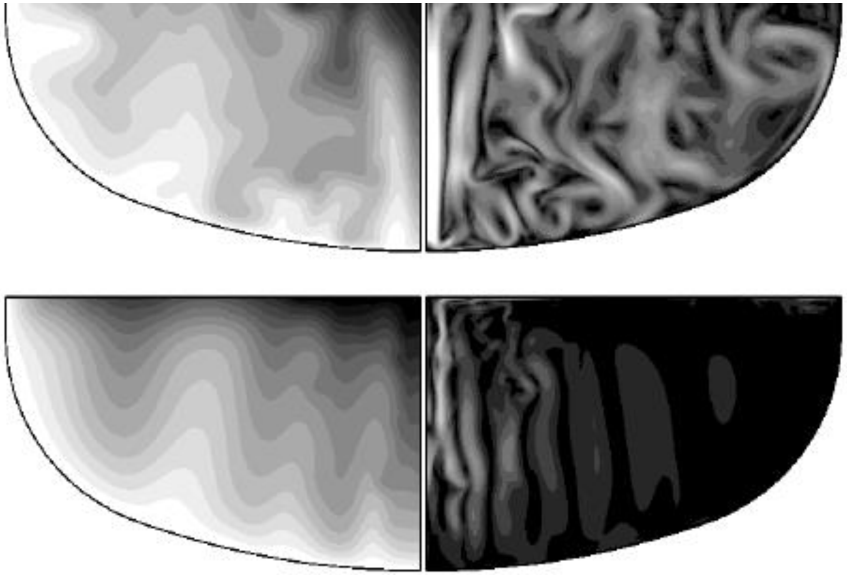
- Navier-Stokes (2D & 3D)
  - Nonnewtonian models
  - Slip coefficients
- RANS turbulence models
  - *SST k-Ω*
  - k-ε
  - v^2-f
- Large eddy simulation (LES)
  - Variational multiscale method (VMS)
- Reynolds equation
  - Dimensionally reduced N-S equations for small gaps (1D & 2D)
- Associated numberical 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, default solvers monolithic
  - Stronger in the elliptic regime of N-S i.e. low Re numbers
  - RANS models have often convergence issues

Czockralski Crystal Growth

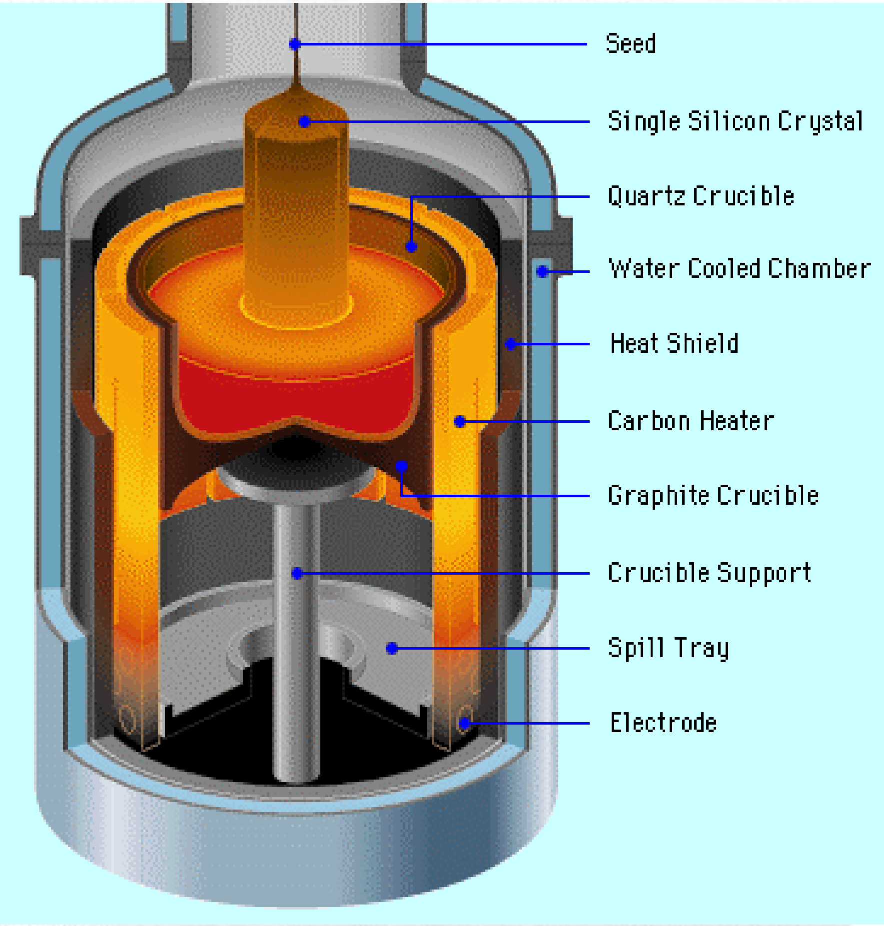
- Most crystalline silicon is grown by the Czhockralski (CZ) method
- One of the key application when Elmer development was started in 1995



Figures by Okmetic Ltd.



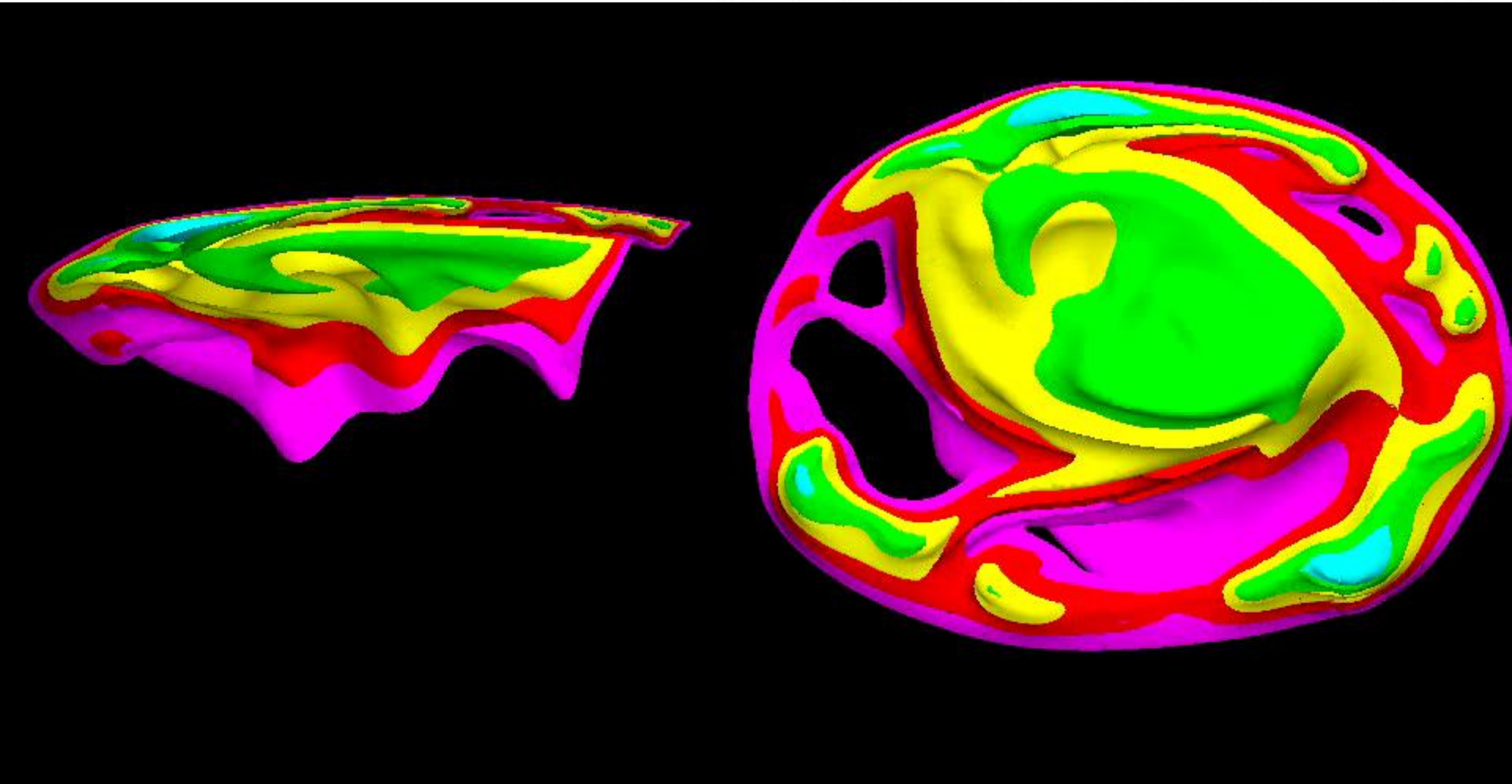
V. Savolainen et al., *Simulation of large-scale silicon melt flow in magnetic Czochralski growth,* J. Crystal Growth 243 (2002), 243-260.



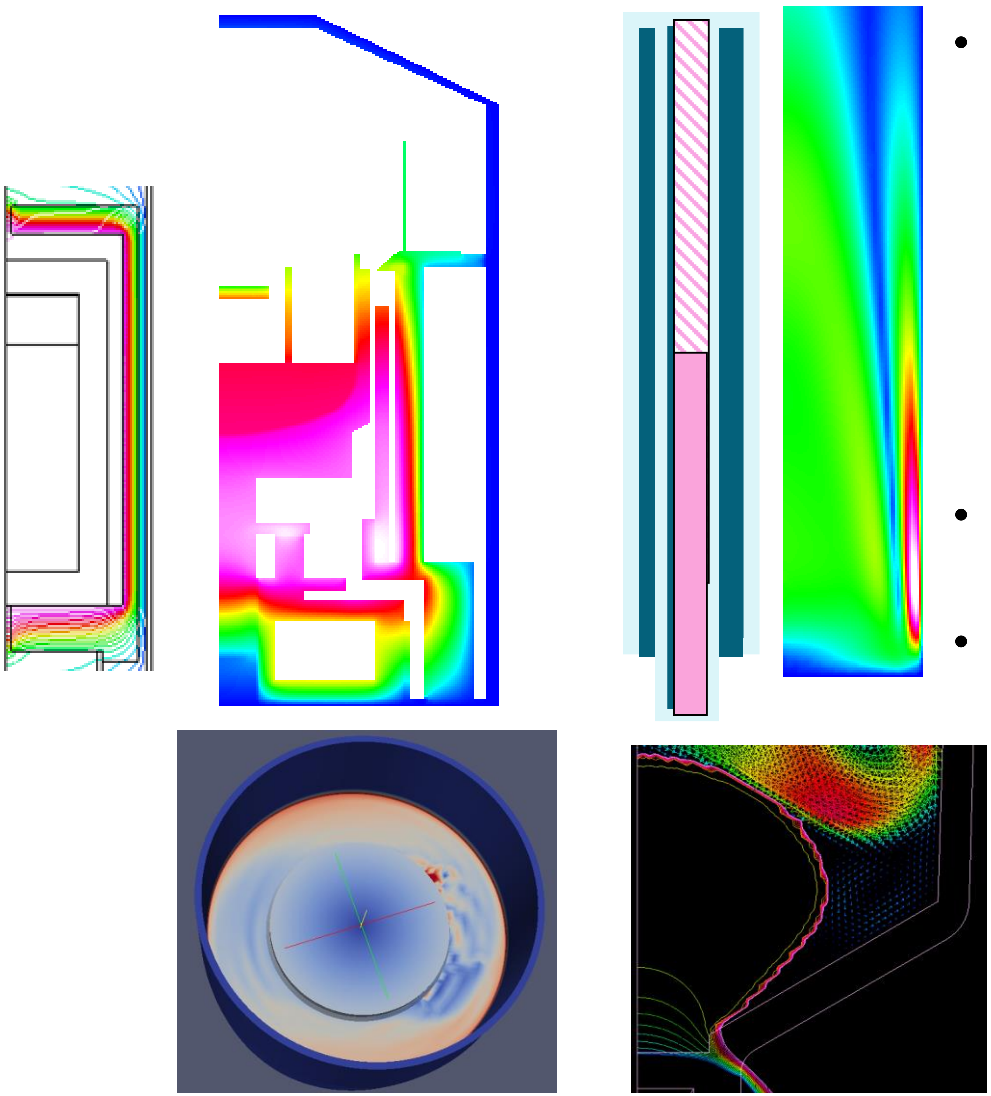
CZ-growth: Transient simulation

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

Simulation Juha Ruokolainen, animation Matti Gröhn, CSC



Elmer in Crystal Growth Simulations



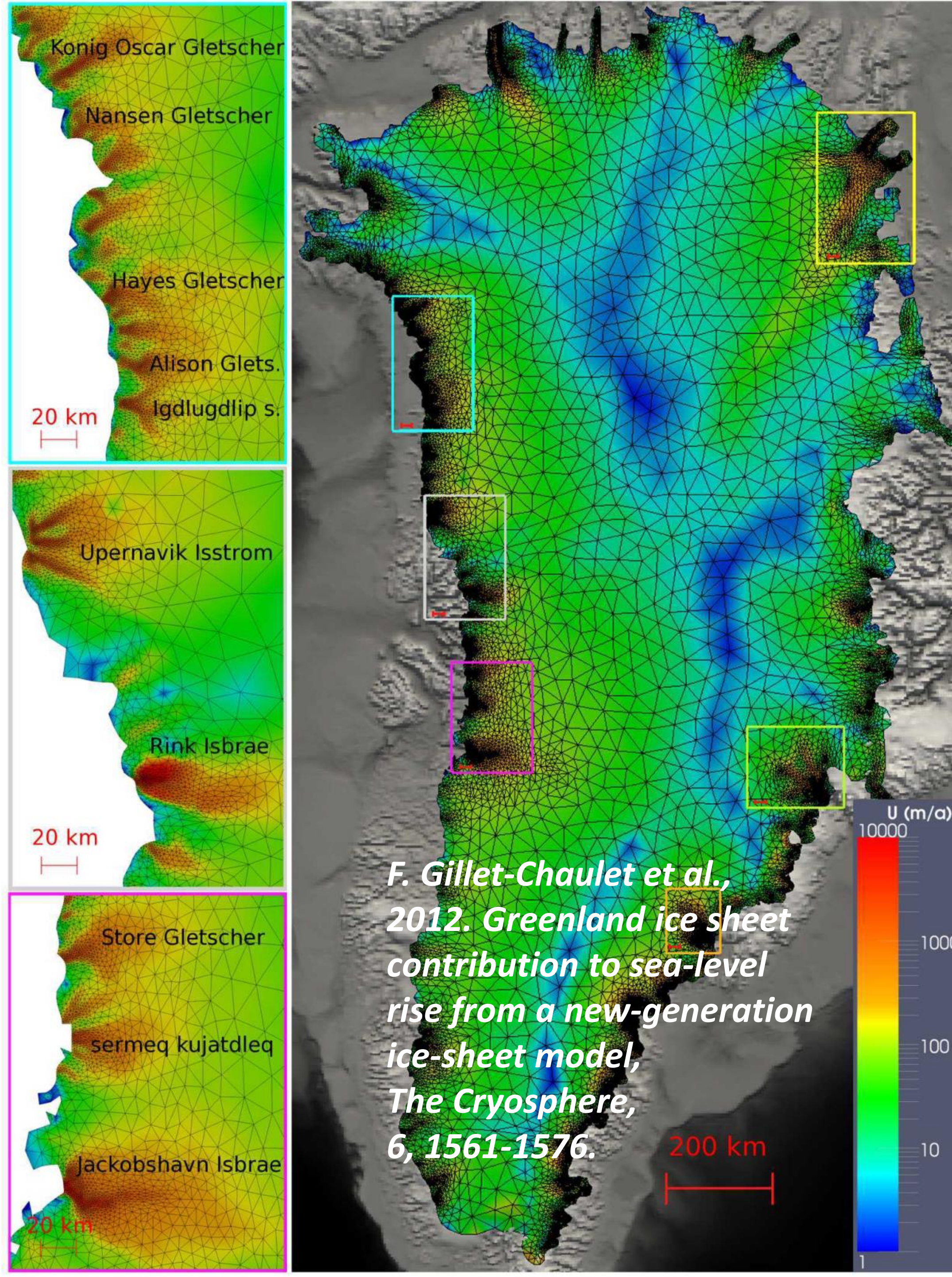
- Elmer has been used extensively in crystal growth simulations: These include crystal and tube growth for silicon, silicon-carbide, NiMnGa and sapphire in Czochralski, HTCVD, sublimation, Bridgman, Vertical Gradient Freeze and Heat Exchanger Methods.
- Numerical results have been successfully verified 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

Silicom

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`**



Thermal creep in light mills

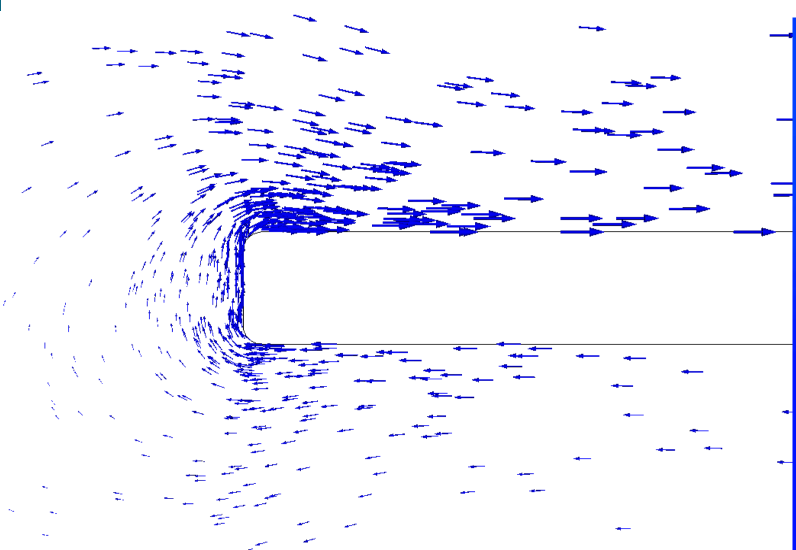
2D compressible Navier-Stokes eq. with heat eq. plus two rarefied gas effects:

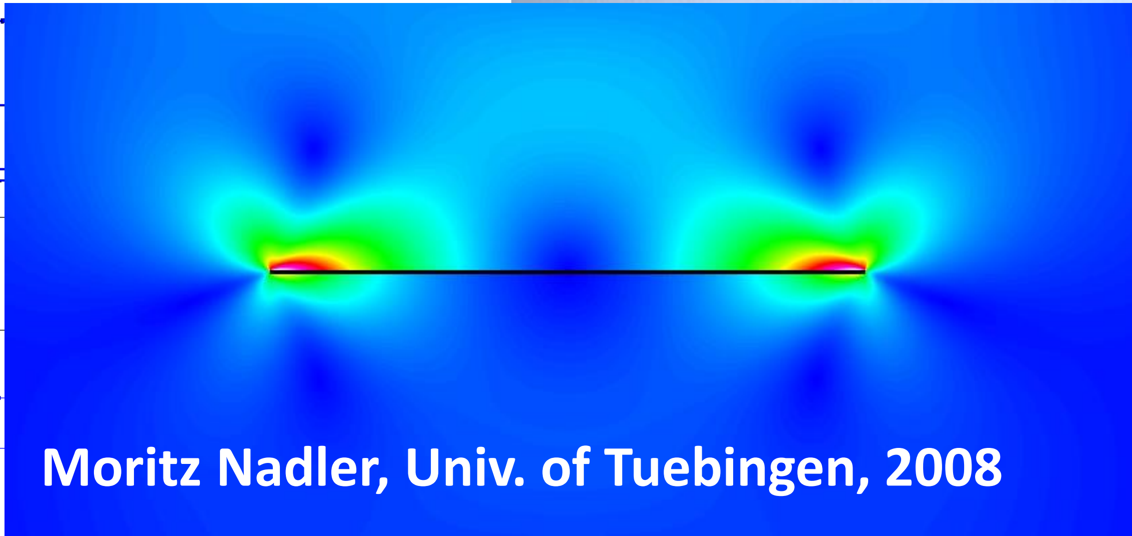
- Maxwell's wall slip and thermal transpiration

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

- Smoluchowski's temperature jump

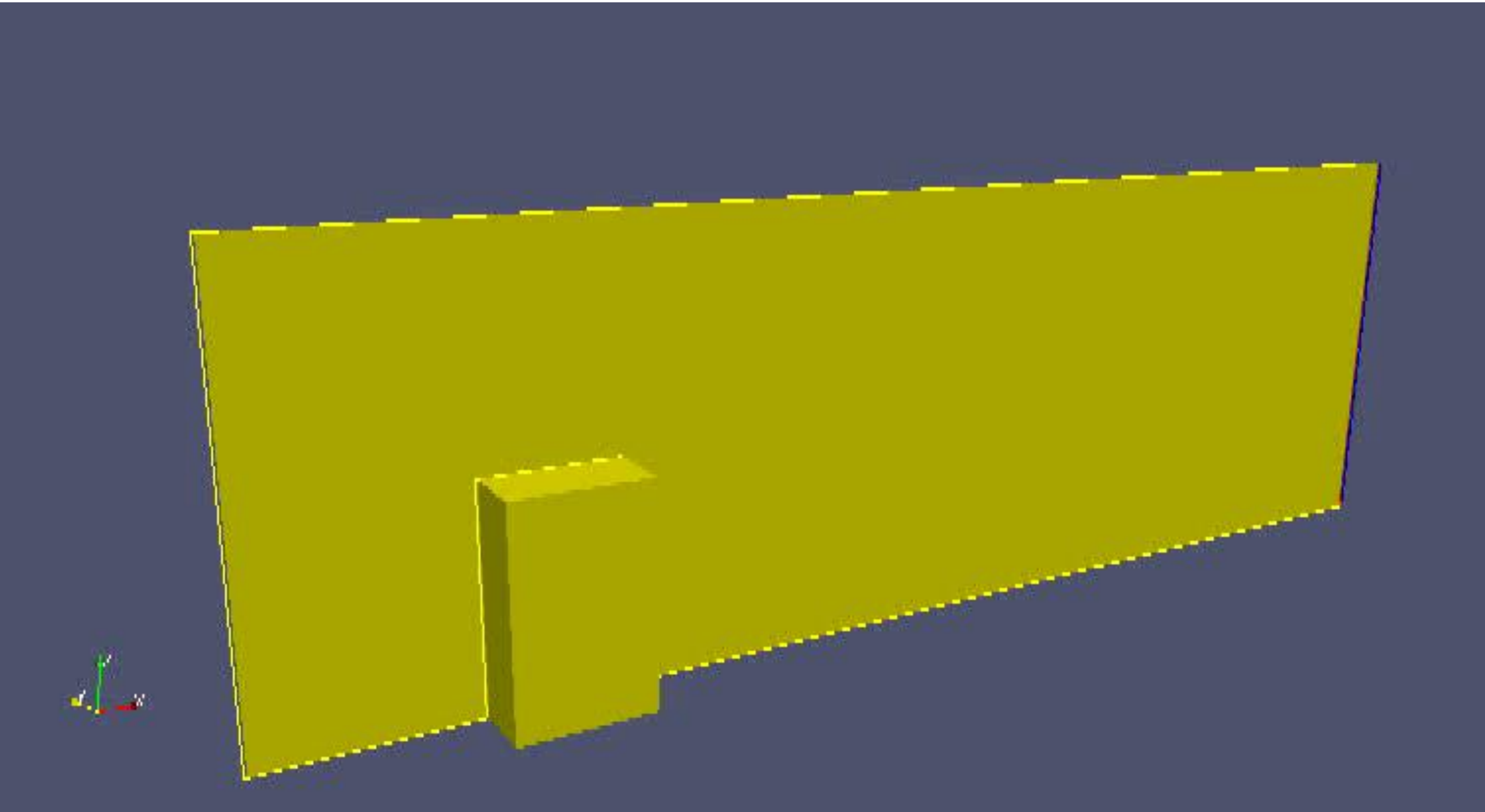
$$T_G - T_W = \frac{2-\sigma_T}{\sigma_T}\frac{2\gamma}{\gamma+1}\frac{\lambda}{Pr}\frac{\partial T}{\partial n}$$





VMS turbulence modeling

- Variational multiscale method (VMS) by Hughes et al. Is a variant of LES particularly suitable for FEM



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 facet shell solver
  - new solver under development
- Some capabilities for contact mechanics

- Associated numerical features
  - Steady-state, harmonic, eigenmode
  - Contact mechanics
- Typical physical coupling
  - Fluid-Structure interaction (FSI)
  - Thermal stresses
  - Source for acoustics
- Known limitations
  - Limited selection of material laws
  - Generality of the contact mechanics

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

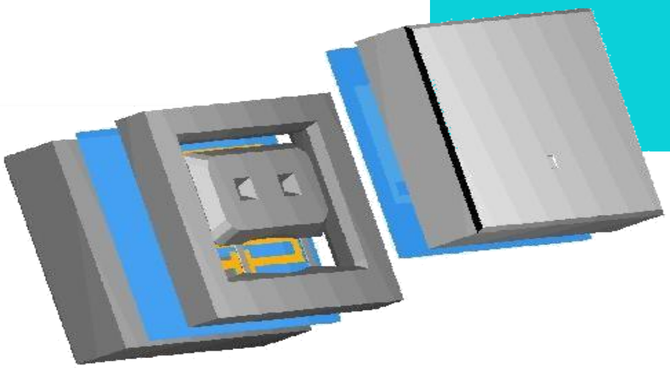
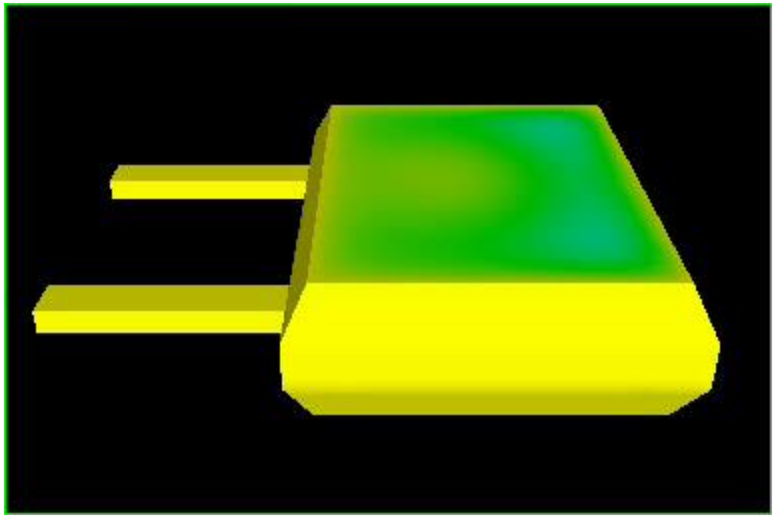
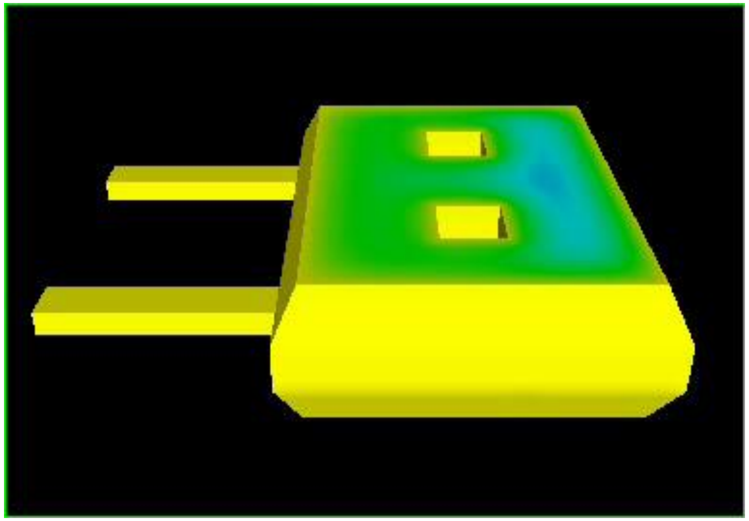


Figure by VTI Technologies

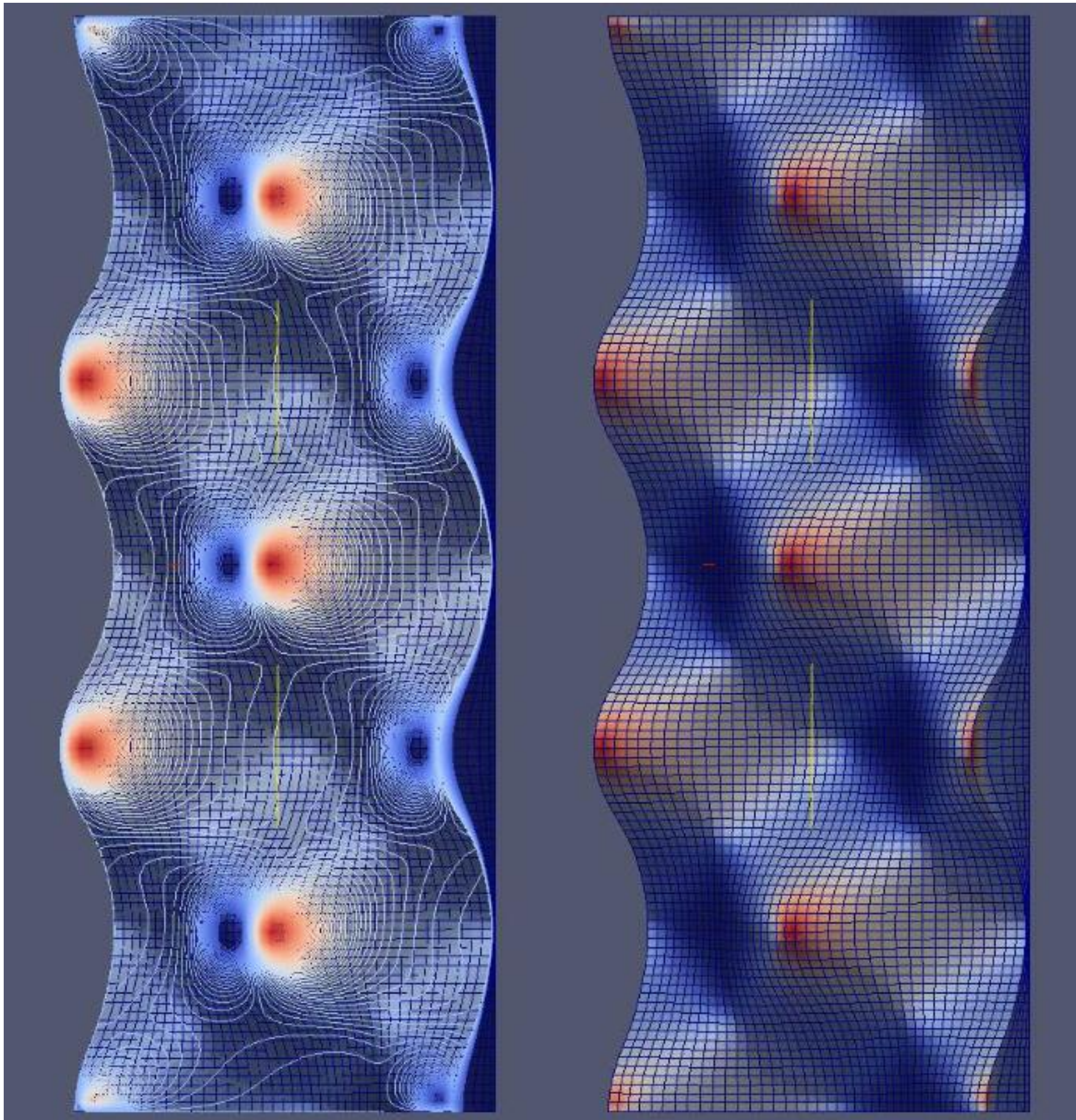




A. Pursula, P. Råback, S. Lähteenmäki and J. Lahdenperä, *Coupled FEM simulations of accelerometers including nonlinear gas damping with comparison to measurements*,
J. Micromech. Microeng. **16** (2006), 2345-2354.

EHDL of patterned surfaces

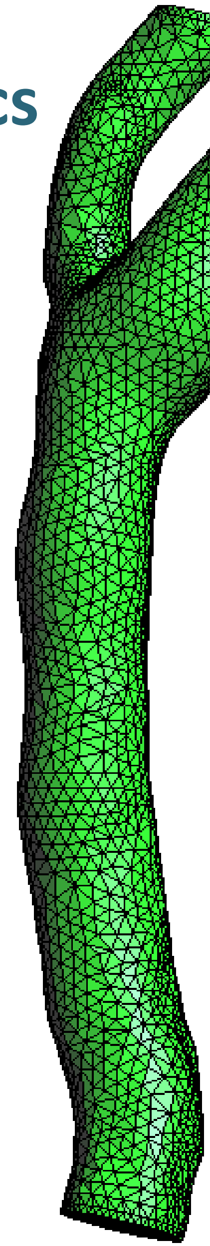
- Solution of Reynolds & nonlinear elasticity equations
- Simulation Bengt Wennehorst, Univ. Of Hannover, 2011

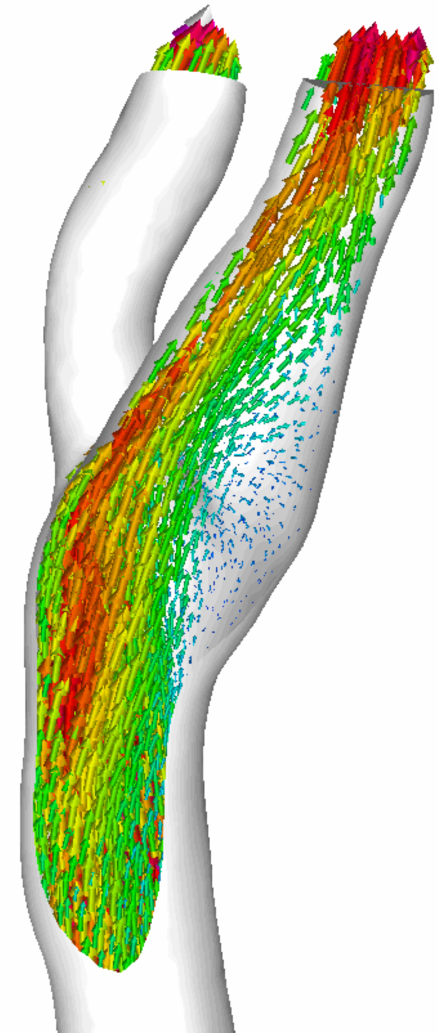


Computational Hemodynamics

- 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

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





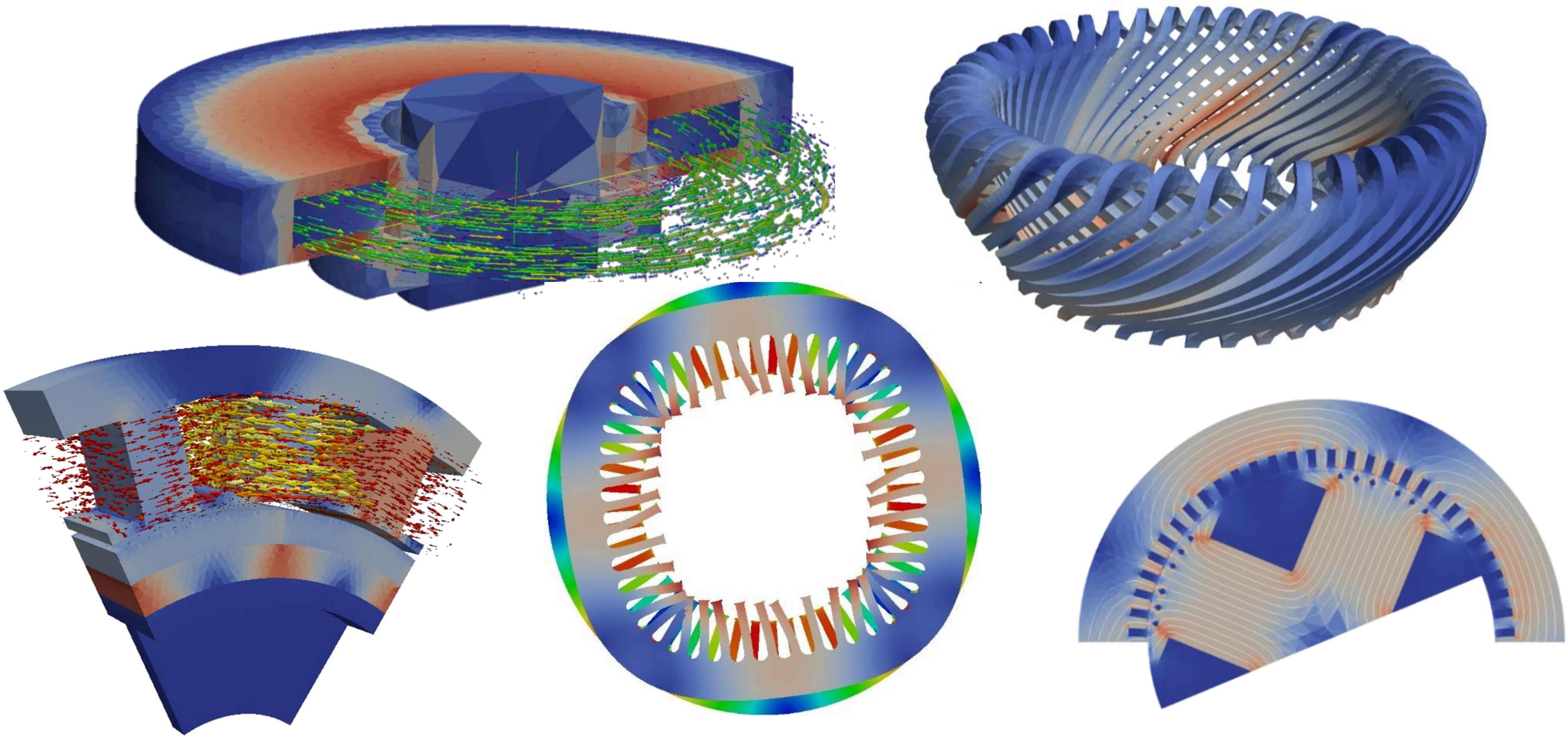
Blood flow in carotid artery accounting FSI interaction

Elmer – Electromagnetics

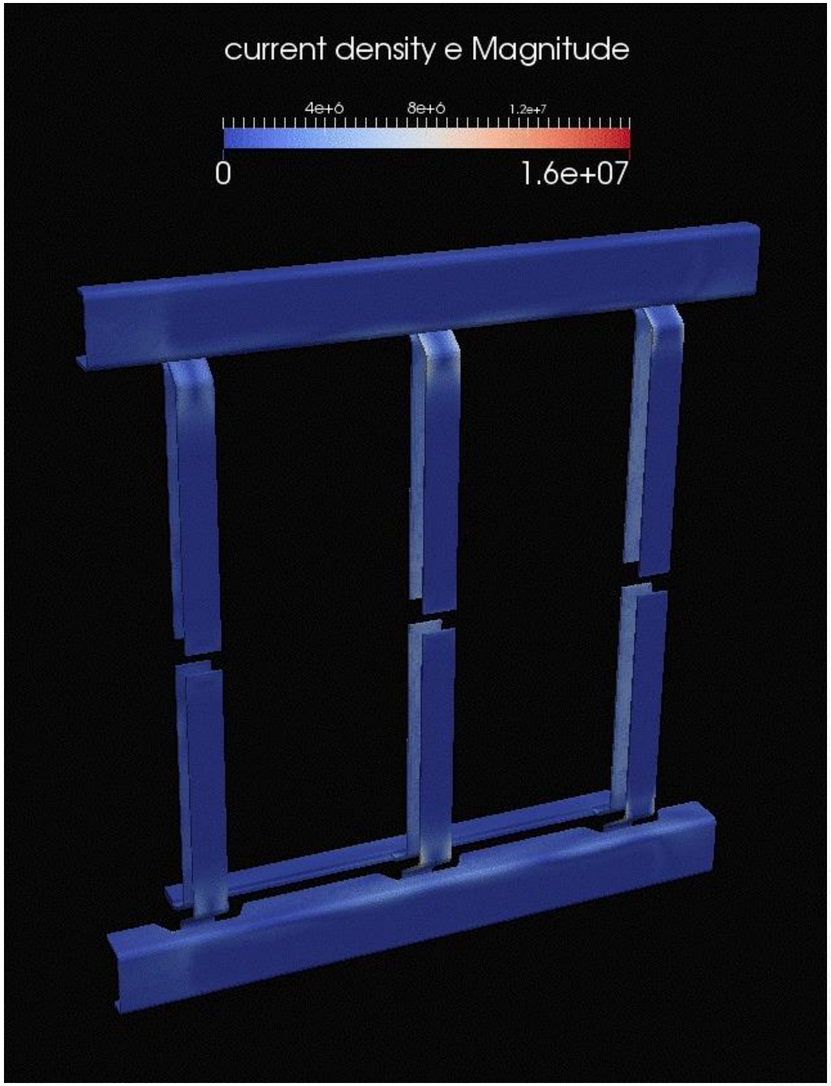
- StatElecSolve for insulators
  - Computation of capacitance matrix
  - Dielectric surfaces
- StatCurrentSolve for conductors
  - Computation of Joule heating
  - Beedback for desired heating power
- Magnetic induction
  - Induced magnetic field by moving conducting media (silicon)
- MagnetoDynamics2D
  - Applicable also to rotating machines
- **MagnetoDynamics3D**
  - Modern AV formulation utilizing edge-elements (1st and 2nd order)
  - Steady-state, harmonic, transient
- VectorHelmholtzSolver
  - Solver for the electromagnetics wave equation
- 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)
  - Electromechanics
- Known limitations
  - One needs to be weary with the Coulomb gauge in some solvers

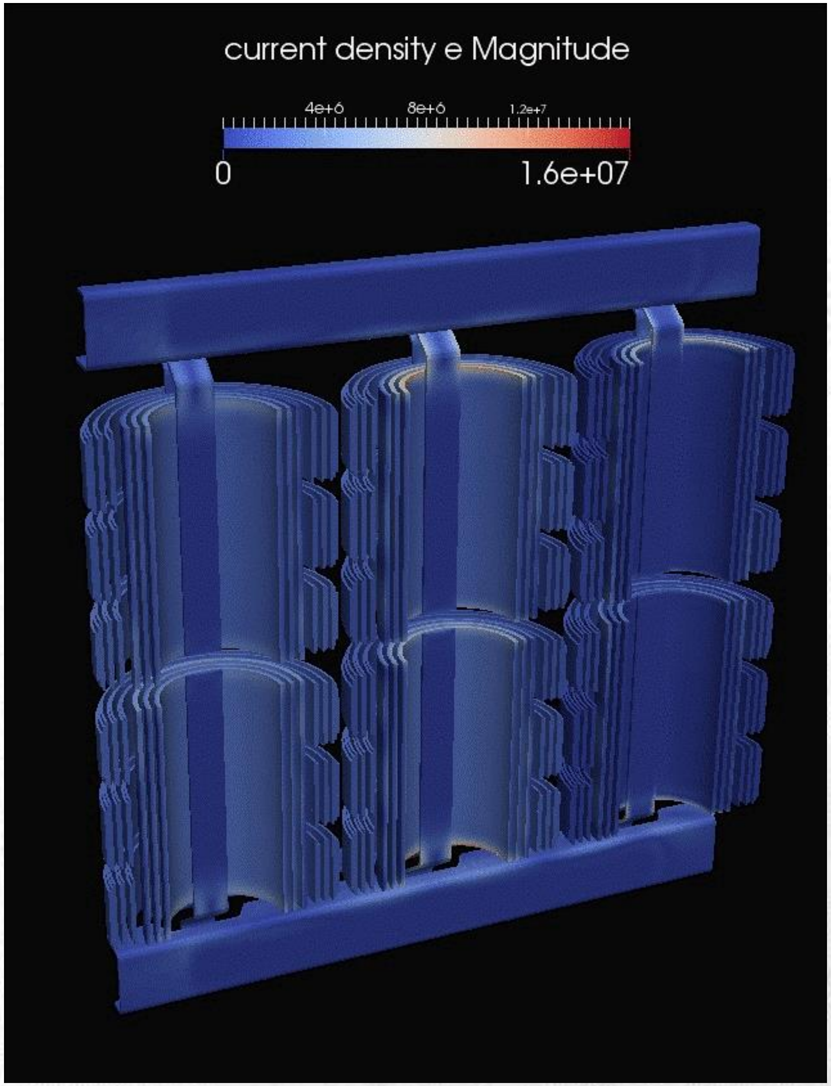
Simulation of electrical machines

- New developmets enable simulation of electrical machines
- Partners: ABB, CSC, Ingersoll-Rand, Kone, Konecranes, Skanveir, Sulzer, Trafotek, Aalto University, LUT, TUT, VTT, (Kuava)



Modeling of magnetic losses in transformers





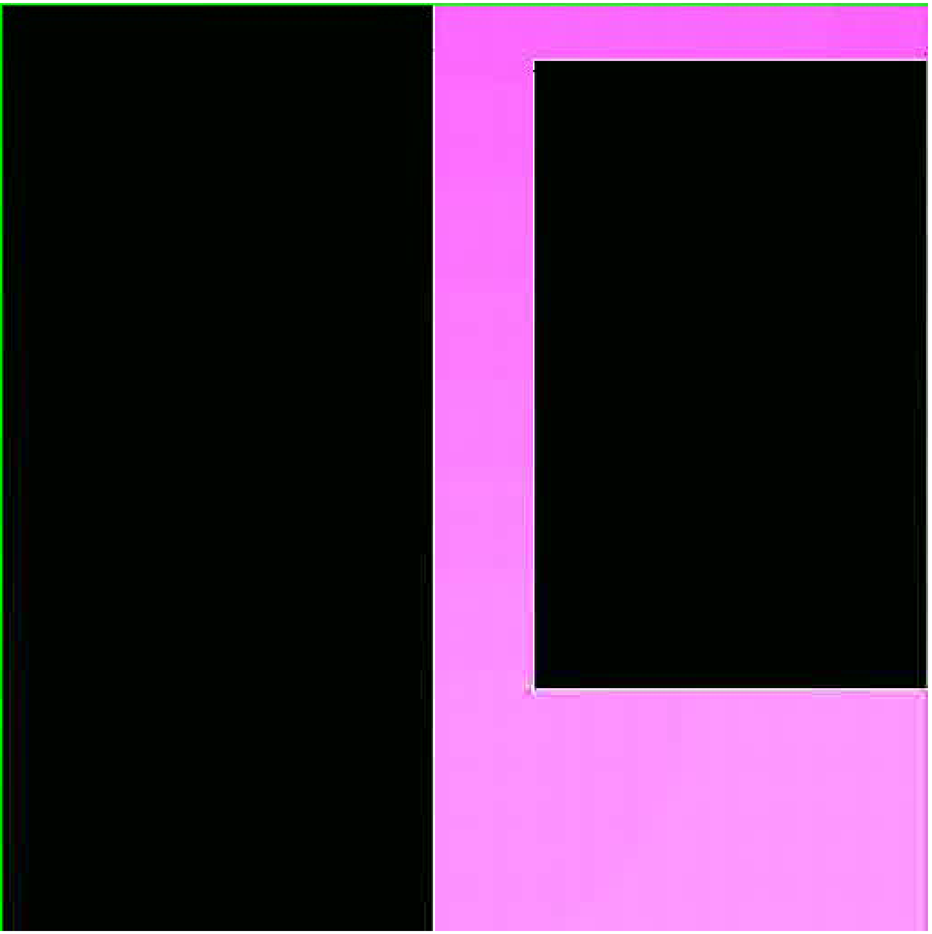
Simulation by Eelis Takala, Trafotek, Finland, 2014

Elmer – Acoustics

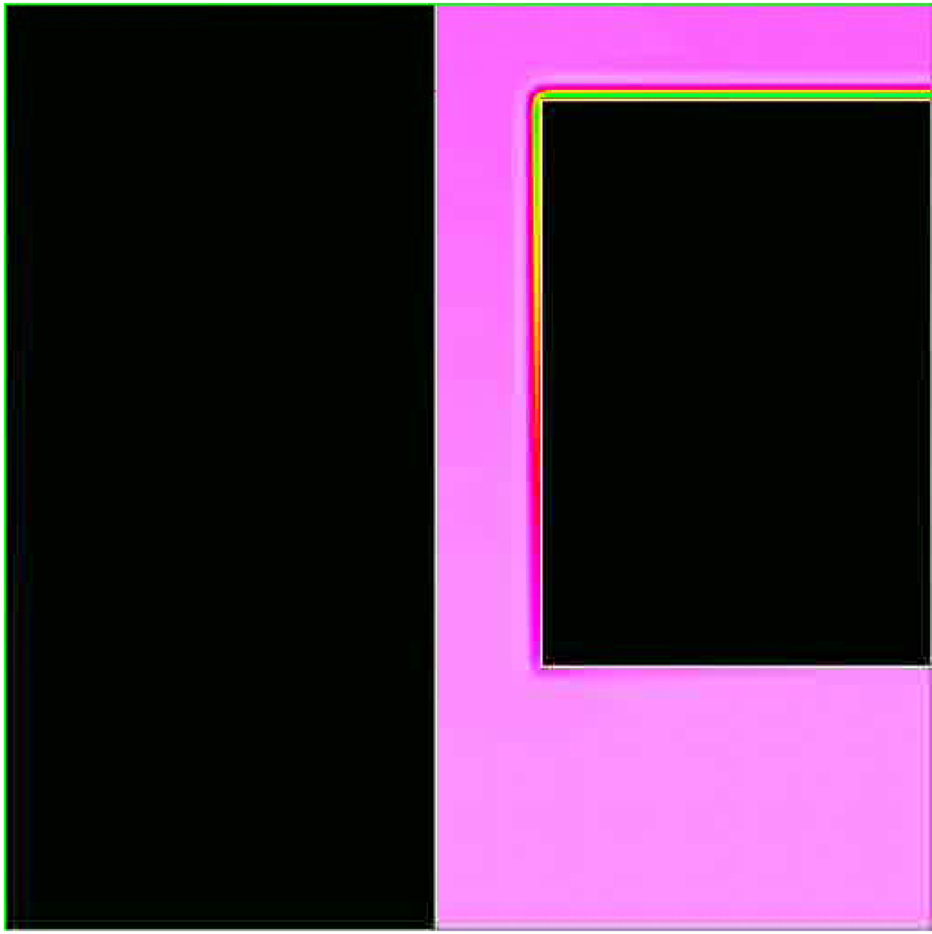
- Helmholtz Solver
  - Possibility to account for convection
- Linearized time-harmonic Navier-Stokes
  - Special equation for the dissipative acoustics
- Thermal Navier-Stokes
  - Ideal gas law
  - Propagation of large amplitude acoutic signals
- Associated numerical features
  - Bubble stabilization
- Typical physical couplings
  - Structural (vibroacoustics)
- Known limitations
  - Limited to small wave numbers
  - N-S equations are quite computitionally intensive

Acoustics: Losses in small cavities

Temperature waves resulting from the Helmholtz equation



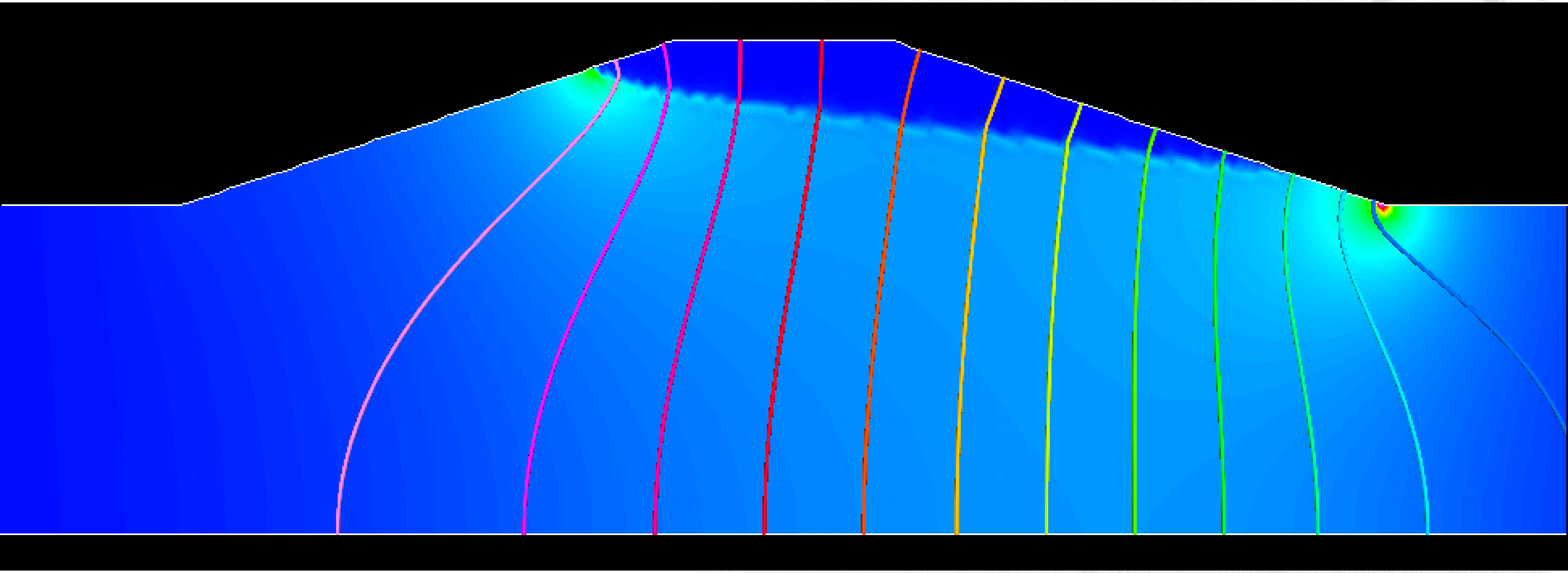
Temperature waves computed from the linearized Navier-Stokes equation



Mika Malinen, *Boundary conditions in the Schur complement preconditioning of dissipative acoustic equations*, SIAM J. Sci. Comput. 29 (2007)

Richard’s equation

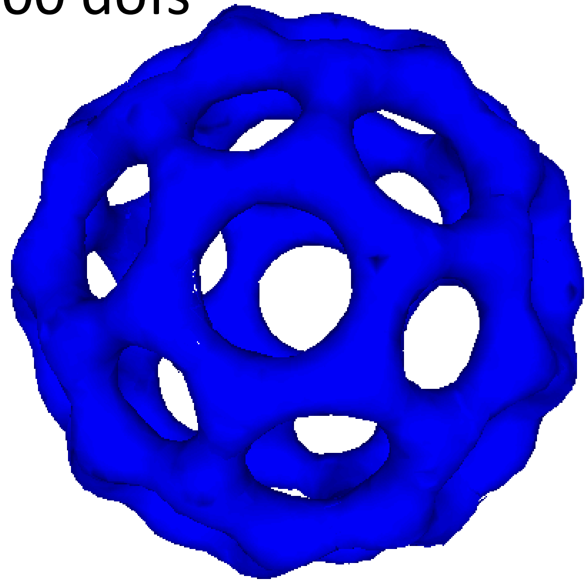
- Richards equations describes the flow of water in the ground
- Porous flow of variably saturated flow
- Modeled with the van Genuchten material models
- Picture show isolines for pressure head and magnitude of the Darcy flux

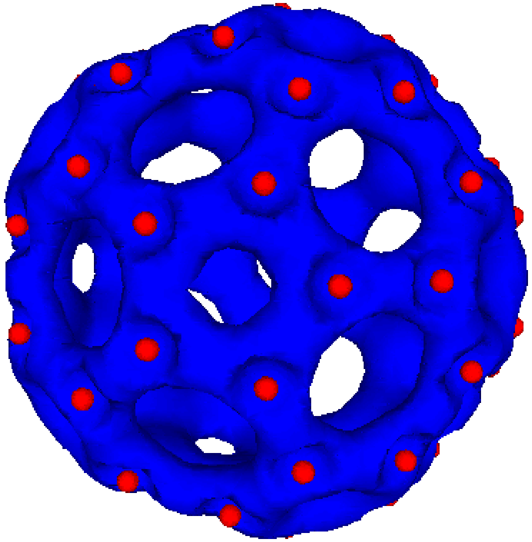


Simulation, Peter Råback, CSC

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 fullerine C60
- All electron computations using 300 000 quadratic tets and 400 000 dofs

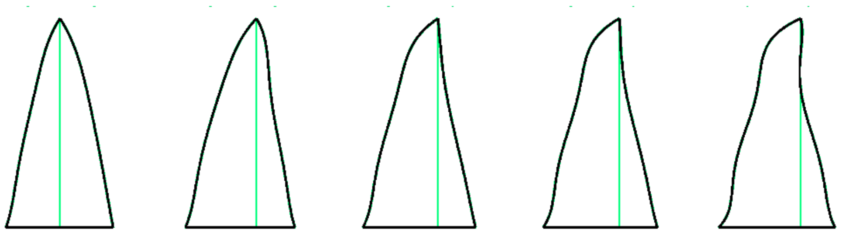




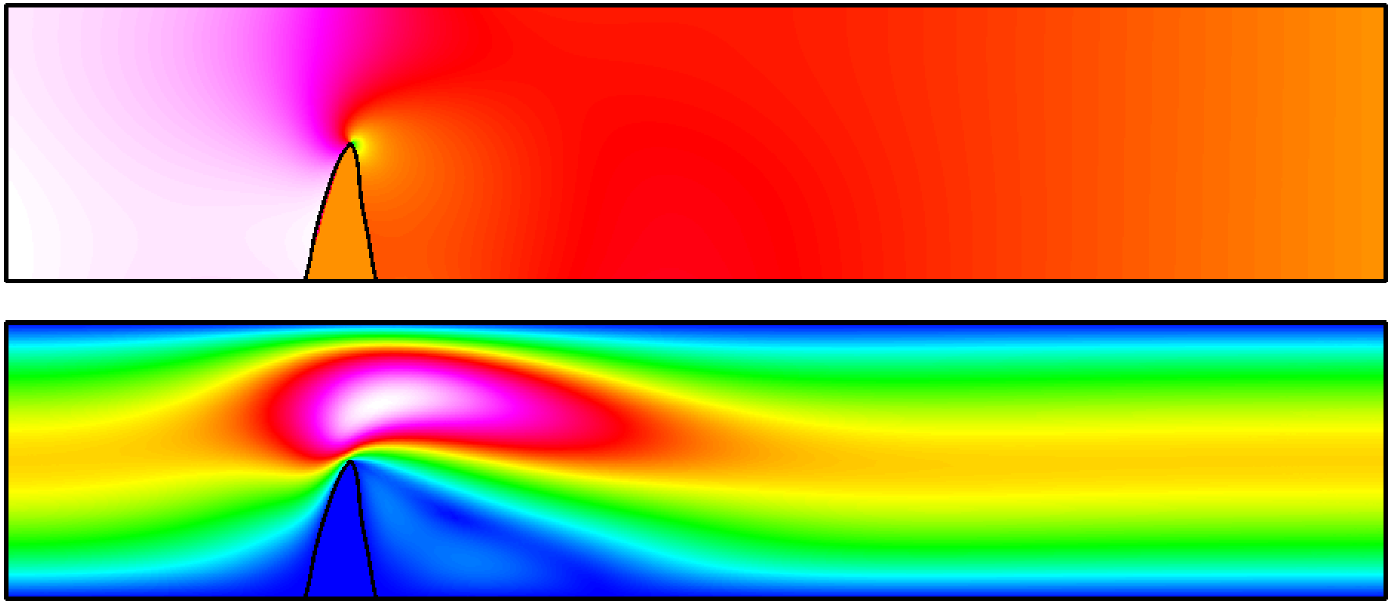
Simulation Mikko Lyly, CSC, 2006

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



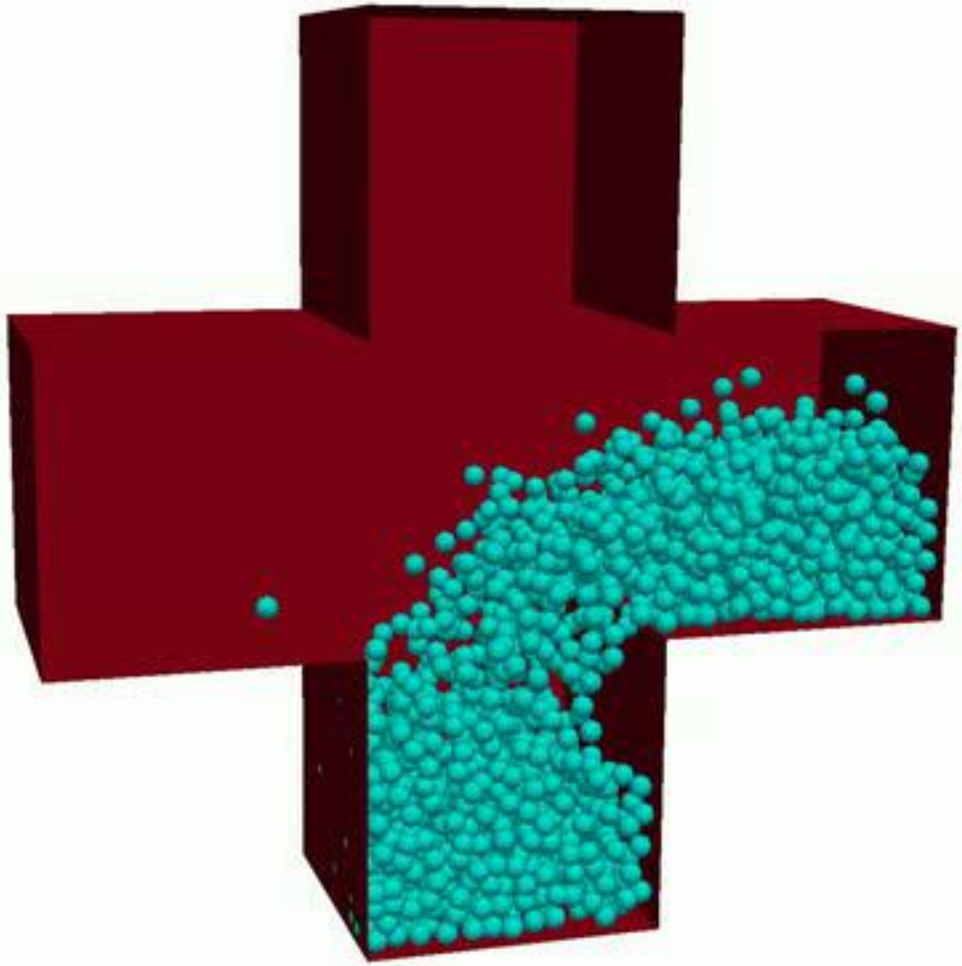
Optimized profiles for Re={0,10,50,100,200}



Pressure and velocity distribution with Re=10

Simulation Peter Råback, CSC

Particle tracker - Granular flow

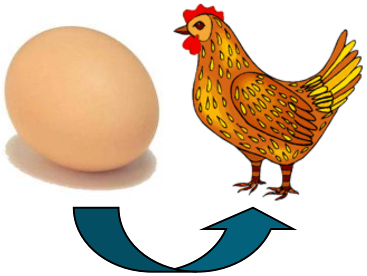


Simulation Peter Råback, CSC, 2011.

Elmer – Selected multiphysics features

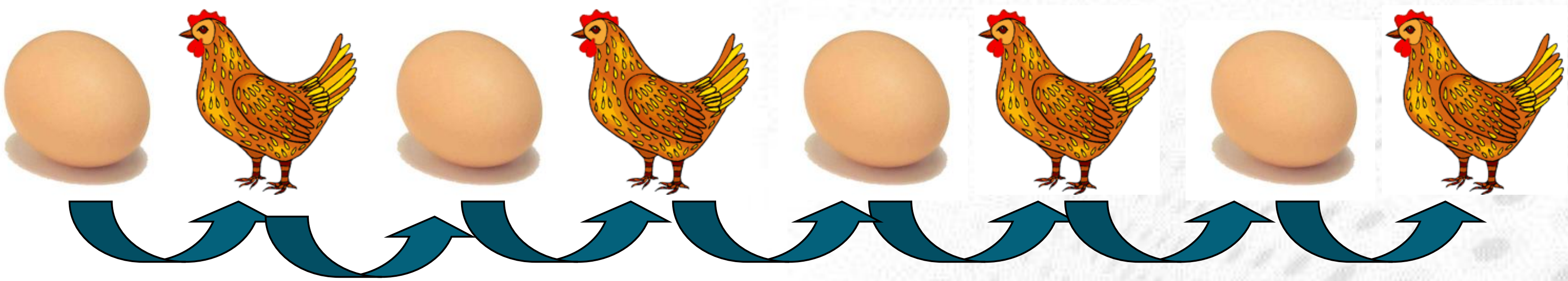
- Solver is an asbtract dynamically loaded object
  - Solver may be developed and compiled without touching the main library
  - No upper limit to the number of Solvers (Currently ~50)
- Solvers may be active in different domains, and even meshes
  - Automatic mapping of field values
- Parameters of 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)

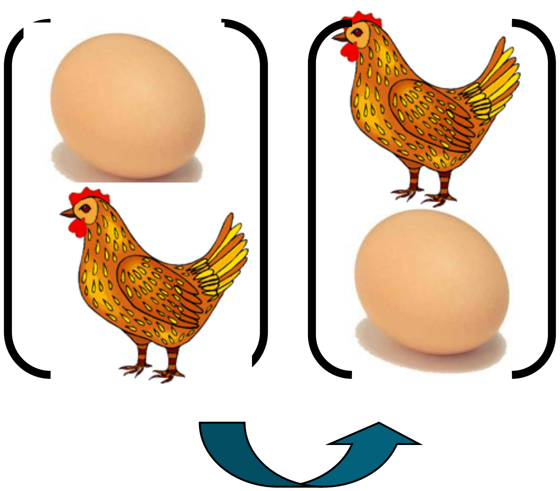
Solution strategies for coupled problems



Hierarchical solution

Iterative solution

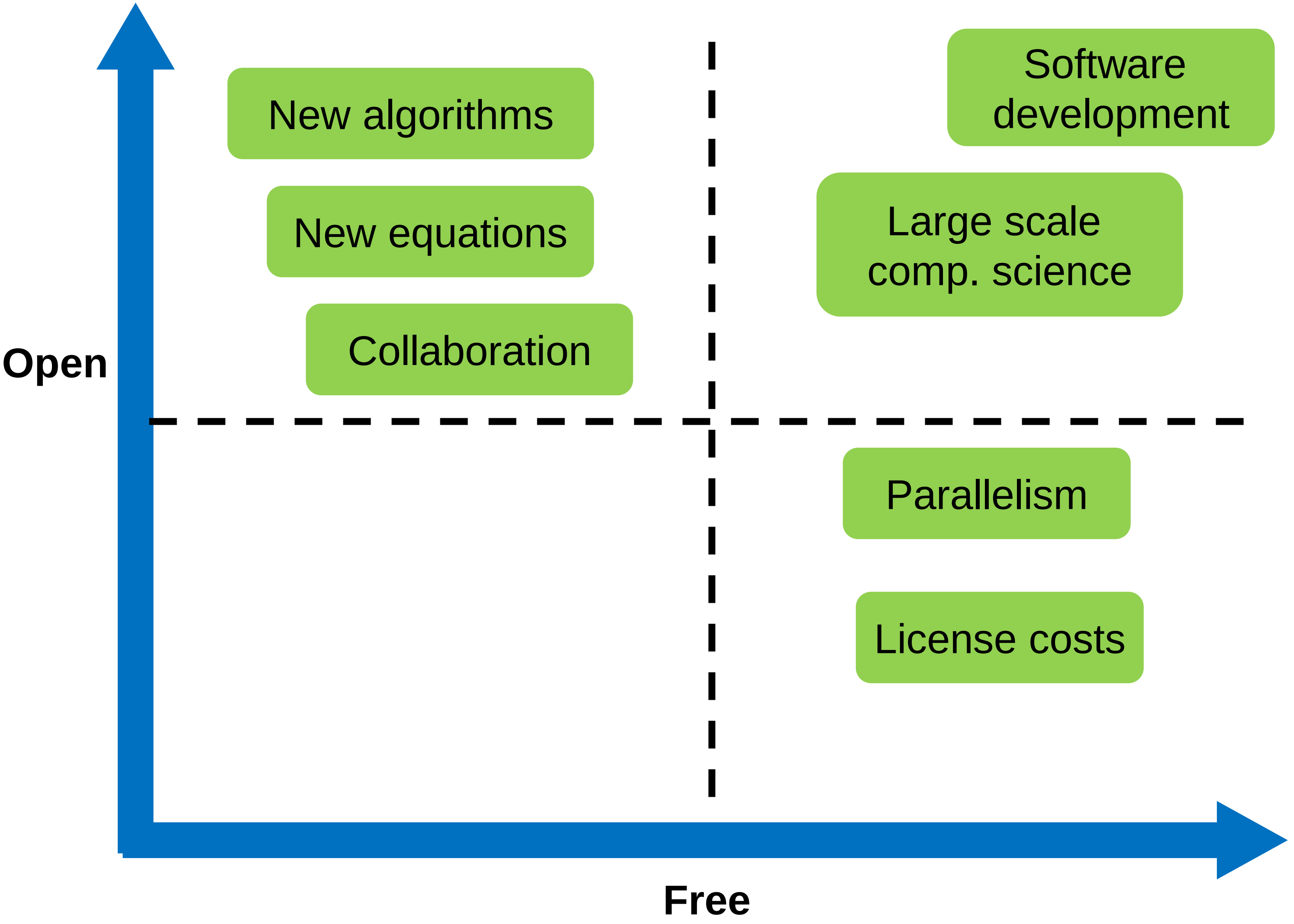




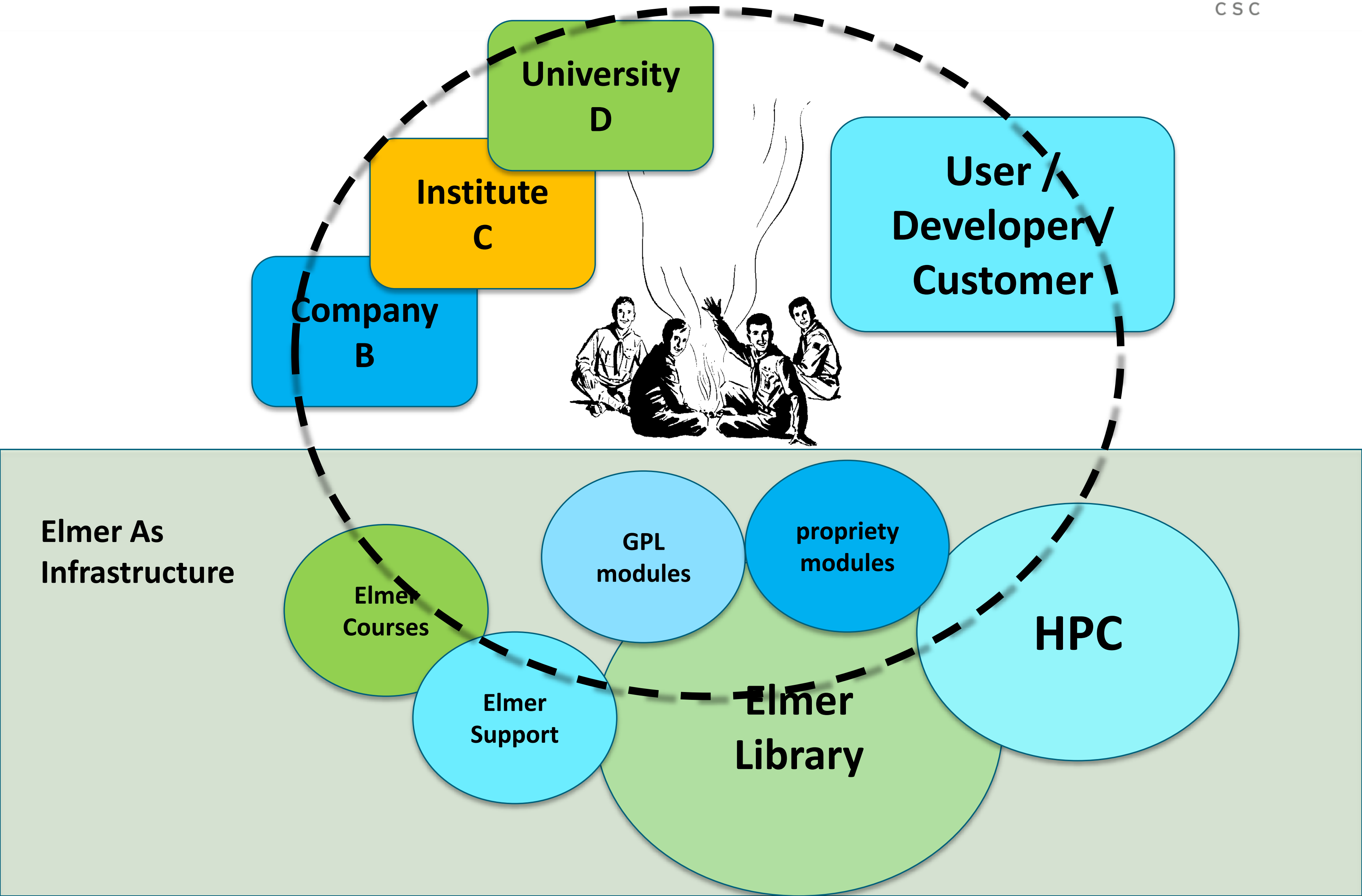
Monolithic solution

Reasons to use open source software in CE

free as in ”beer” vs. free as in ”speech”



Elmer – Infrastructure for Open Research



Most important Elmer resources

- http://www.csc.fi/elmer
  - Official Homepage of Elmer
- http://sourceforge.net/projects/elmerfem/
  - SVN version control system & Windows binaries
- https://github.com/elmercsc/elmerfem
  - GIT version control (the future)
- http://www.elmerfem.org
  - Discussion forum, wiki & doxygen
- http://youtube.com/elmerfem
  - Youtube channel for Elmer animations
- Further information: elmeradm@csc.fi