Elmer

Open Source Finite Element Software for Multiphysical Problems

Peter Råback
ElmerTeam
CSC – IT Center for Science

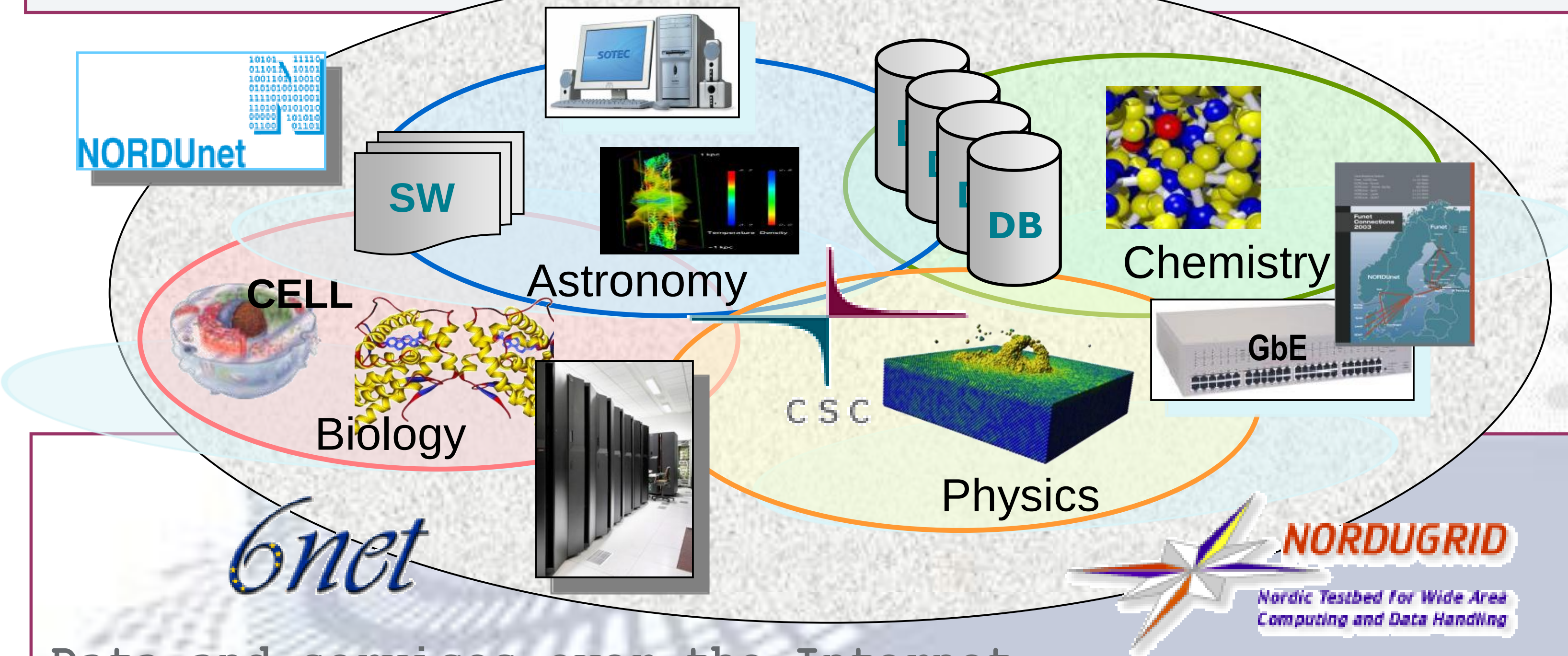
Tampere Univ. of Tech.
24.4.2014

What is CSC?

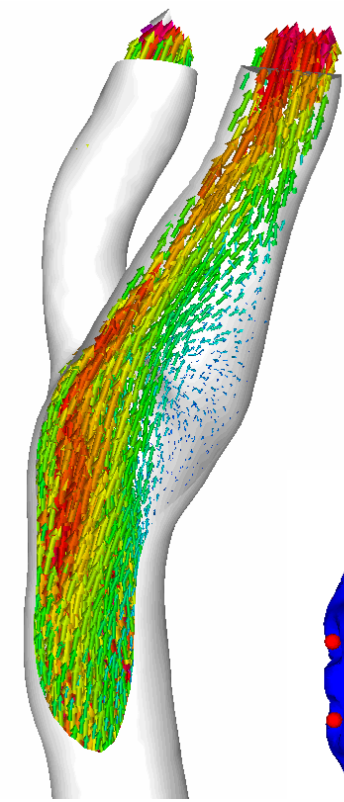
- Founded in 1971 as a technical support unit for Univac 1108
- Connected Finland to the Internet in 1988
- Owned by the Ministry of Education and Culture of Finland
- Operates on a **non-profit** principle
- Facilities in Espoo, close to Otaniemi campus and Kajaani
- Staff ~250
- Currently official name is: ”**CSC – IT Center for Science”**

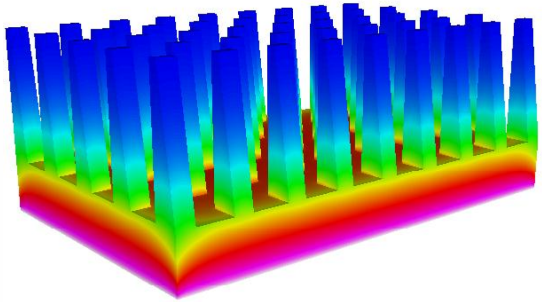
CSC as a Finnish IT Infrastructure for Research

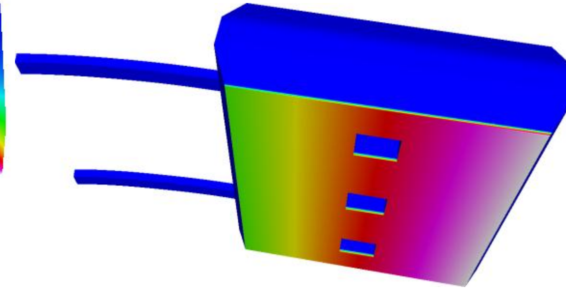
The volume of data is growing exponentially. To exploit the data for, e.g., drug design, a global, constantly updating IT infrastructure is needed (programs, DBs)

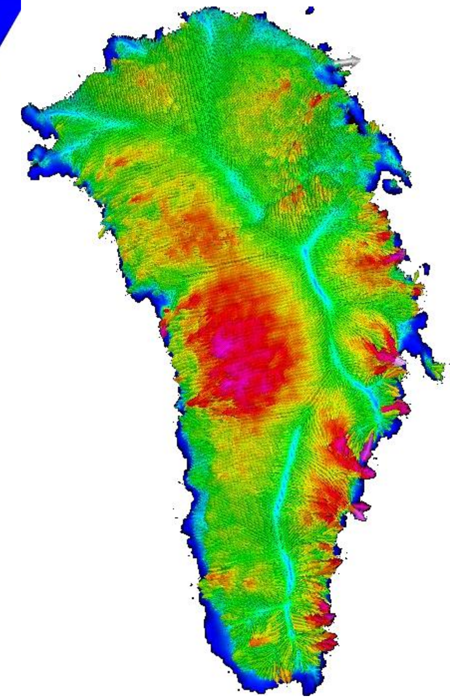


Data and services over the Internet

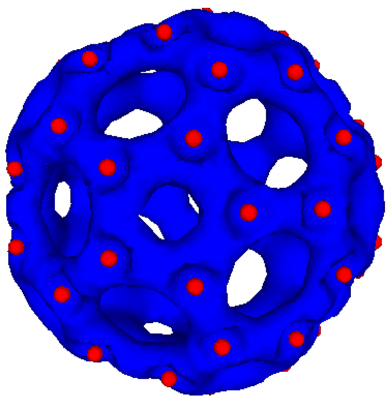


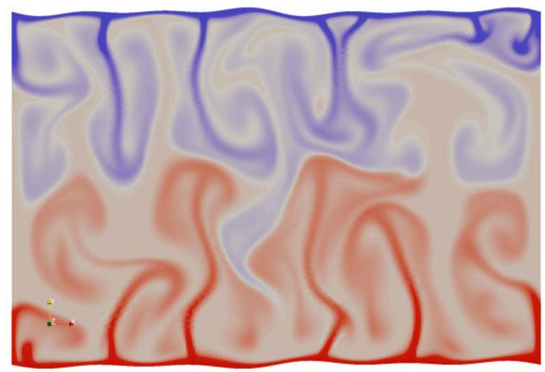


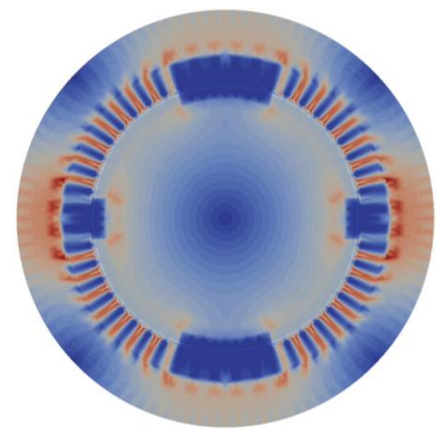


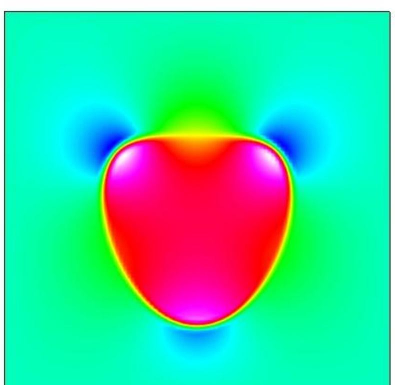


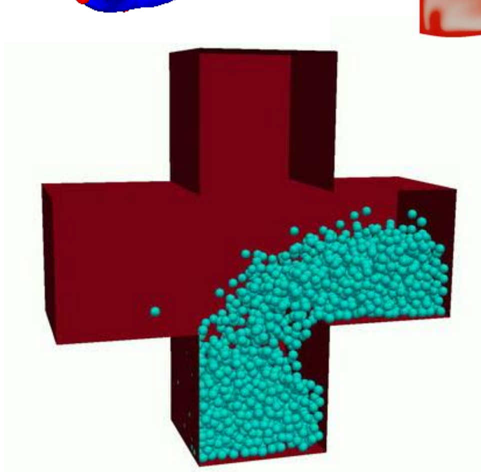
Elmer finite element software for multiphysical problems

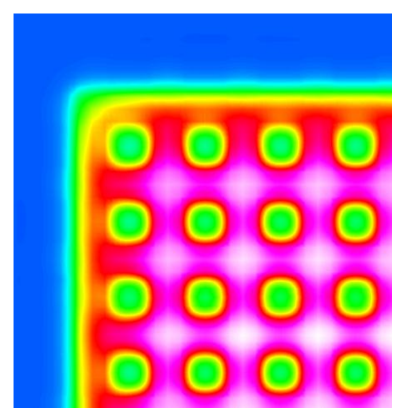












Figures by Esko Järvinen, Mikko Lyly, Peter Råback, Timo Veijola (TKK) & Thomas Zwinger

Short history of Elmer

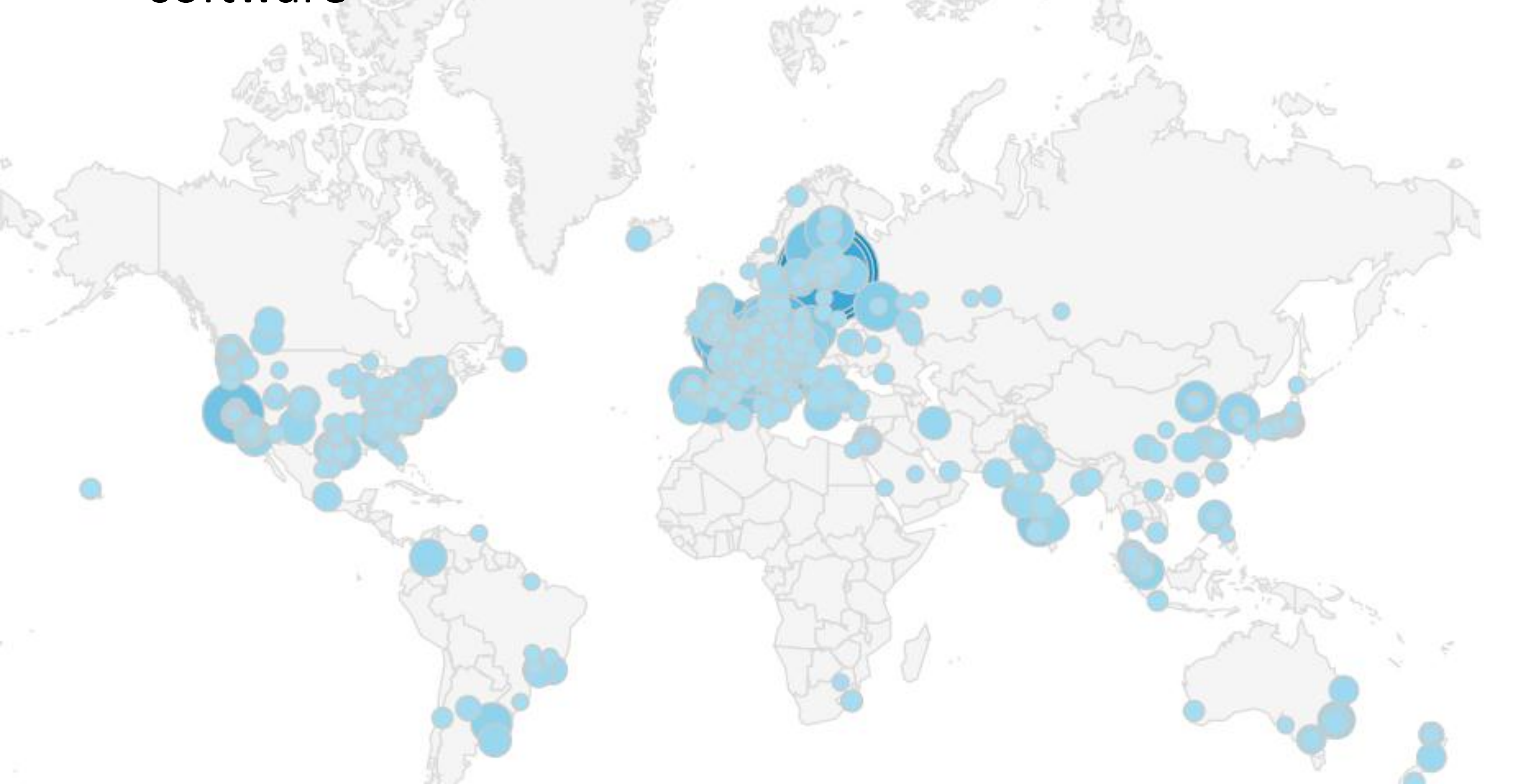
- 1995 Elmer development was started as part of a national CFD program
  - Collaboration of CSC, TKK, VTT, JyU, and Okmetic Ltd.
- 2000 After the initial phase the development driven by number of application projects
  - MEMS, Microfluidics, Acoustics, Crystal Growth, Hemodynamics, Glaciology, …
- 2005 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

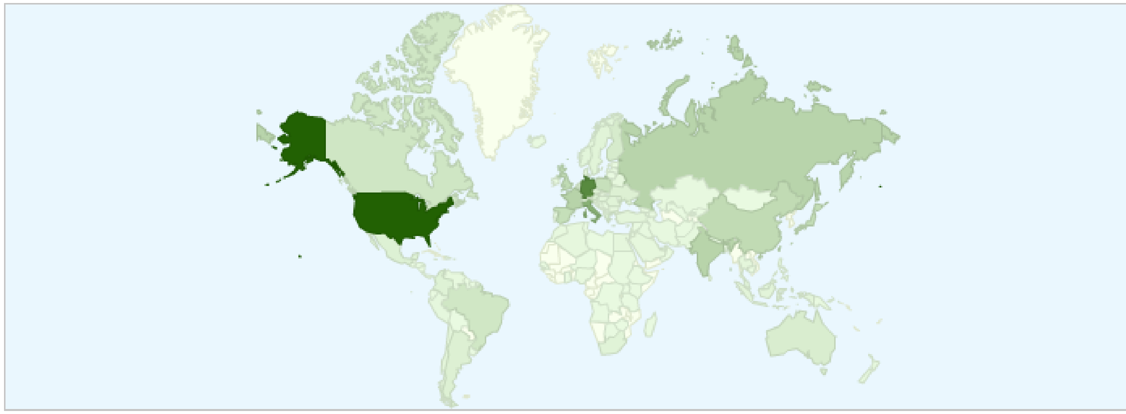
- Used worldwide by thousands of researchers (?)
- One of the most popular open source multiphysical software



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

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

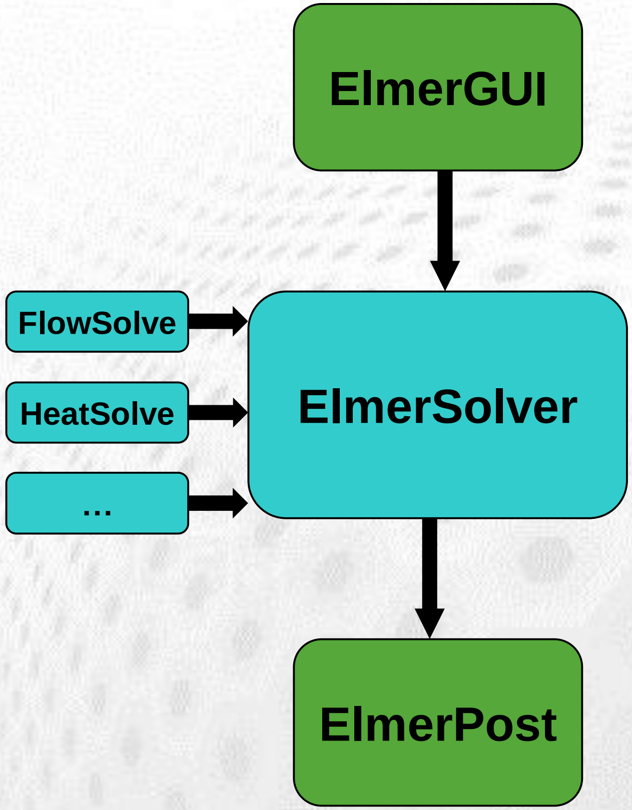
93% of downloaders

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

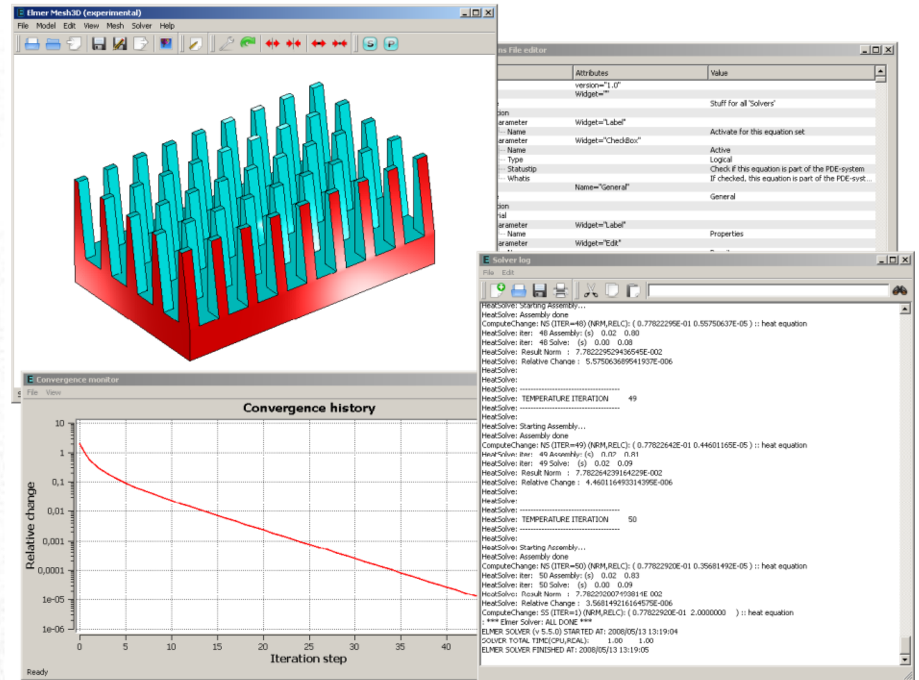
Elmer finite element software

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



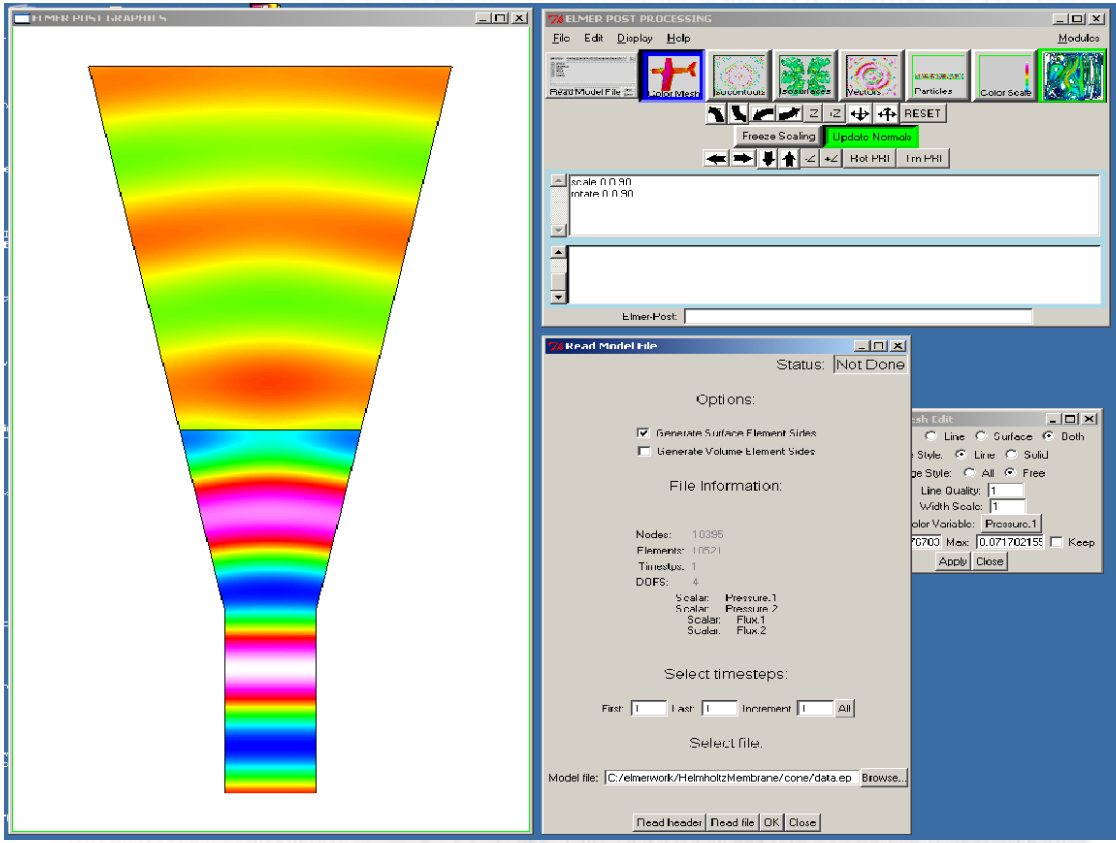
ElmerGUI

- 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



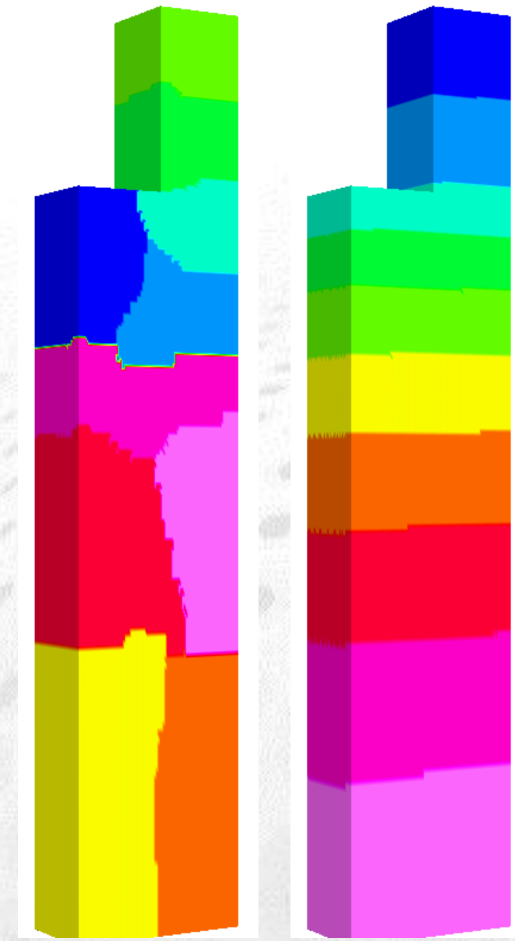
ElmerPost

- 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 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,…)



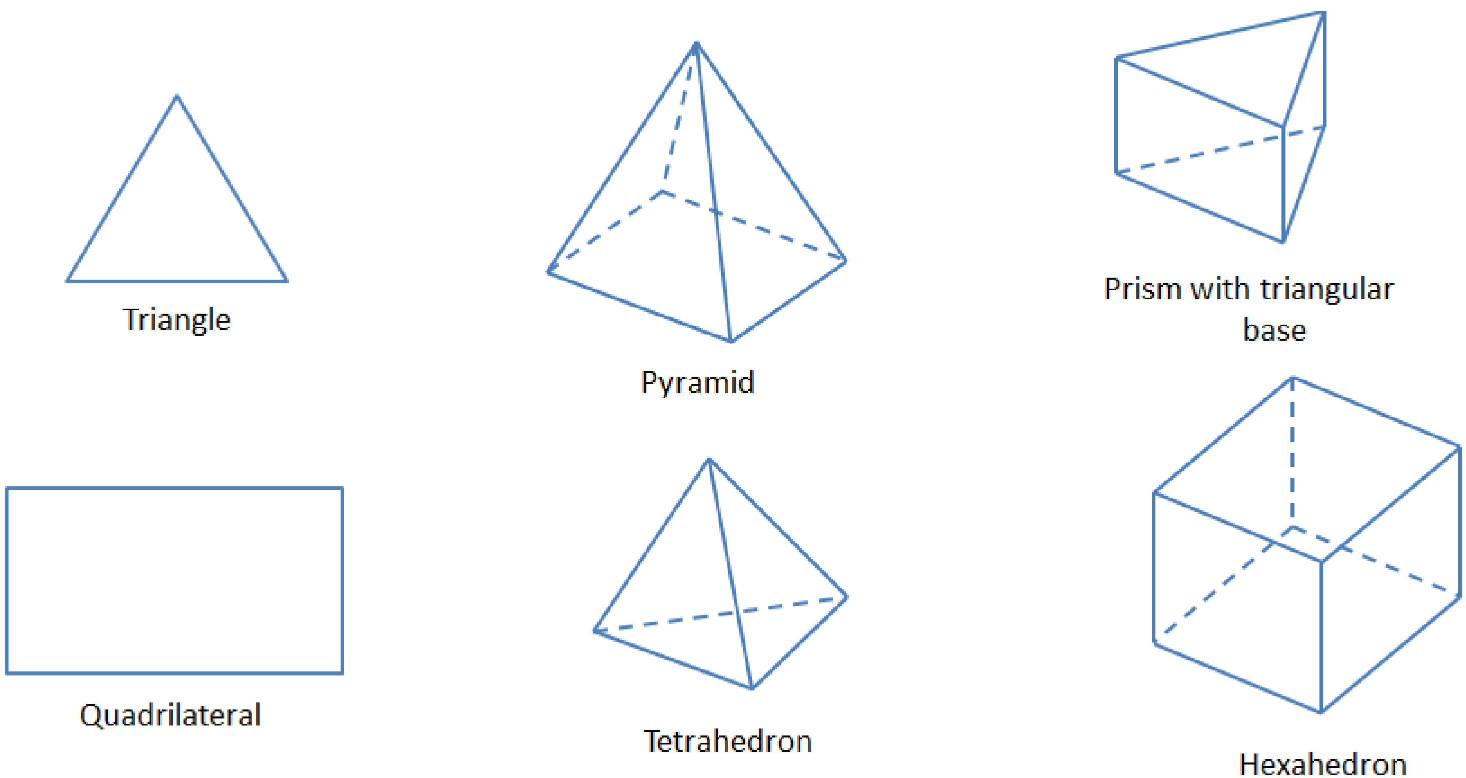
ElmerSolver

- 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
```

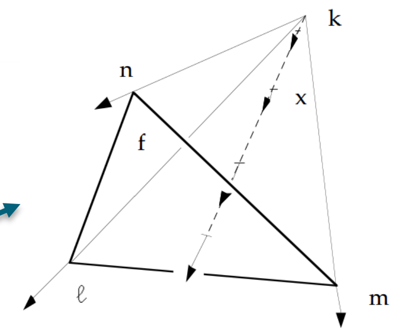
ElmerSolver – Finite element shapes

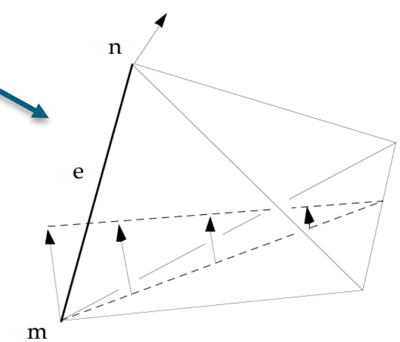
- 0D: vertex
- 1D: edge
- 2D: triangles, quadrilateral
- 3D: tetrahedrons, prisms, pyramids, hexahedrons



ElmerSolver – Finite element basis functions

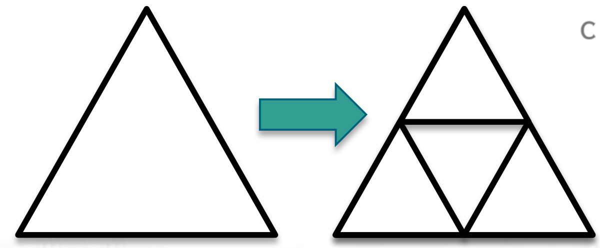
- Element families
  - nodal, DG
  - p-elements
  - edge, face –elements
    - Hdiv (often associated with”face” elements)
    - Hcurl (often associated with ”edge” elements)
- Formulations
  - Galerkin, Discontinuous Galerkin
  - Stabilization
  - Residual free bubbles



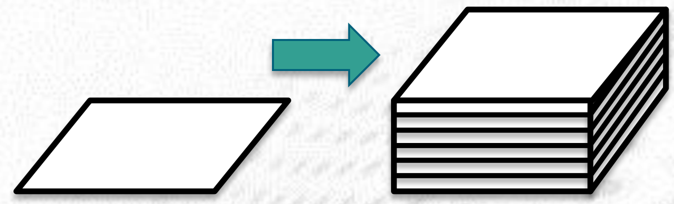


ElmerSolver – meshing features

- 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?

You may select up to **5** options

Heat transfer	✓	64	28%
Fluid mechanics	✓	61	27%
Solid mechanics	✓	47	21%
Electromagnetics		38	17%
Quantum mechanics		3	1%
Something else (please specify)		12	5%

Total votes : 225

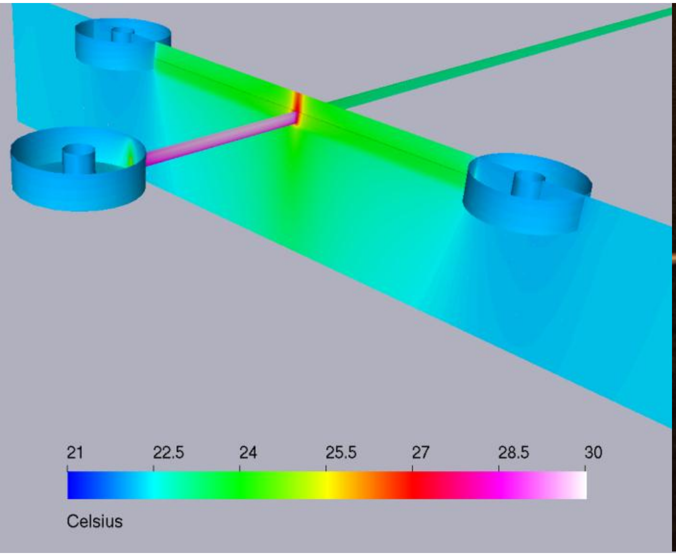
Submit vote

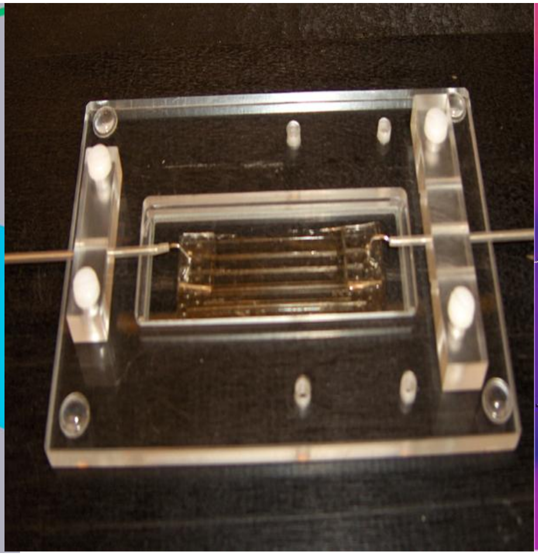
Elmer – Heat Transfer

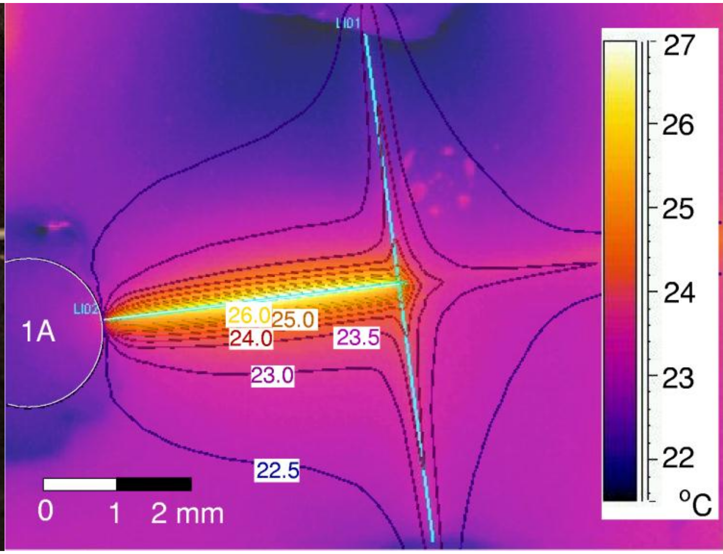
- Heat equation
  - convection
  - diffusion
  - Phase change
  - Temperature control feedback
  - Thermal slip BCs for small Kn number
- Radiation with view factors
  - 2D, axisymmetric use numerical integration
  - 3D based on ray tracing
  - Stand-alone program
- Strongly coupled thermoelectric equation

- 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

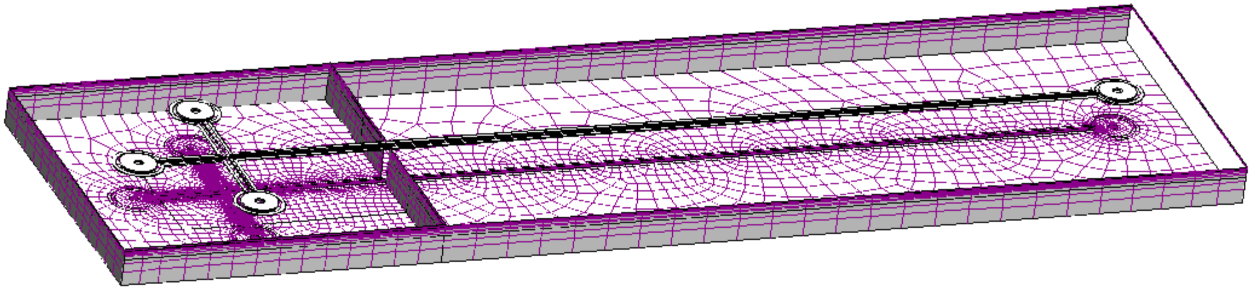
Microfluidics: Flow and heat transfer in a microchip







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



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

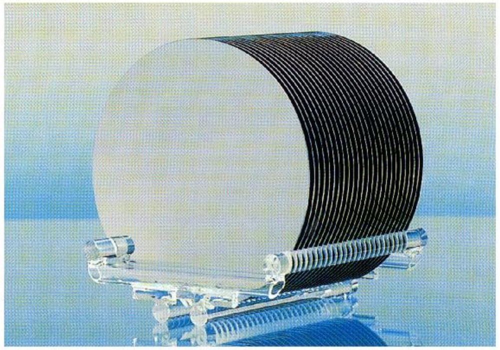
Elmer – Fluid Mechanics

- 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)

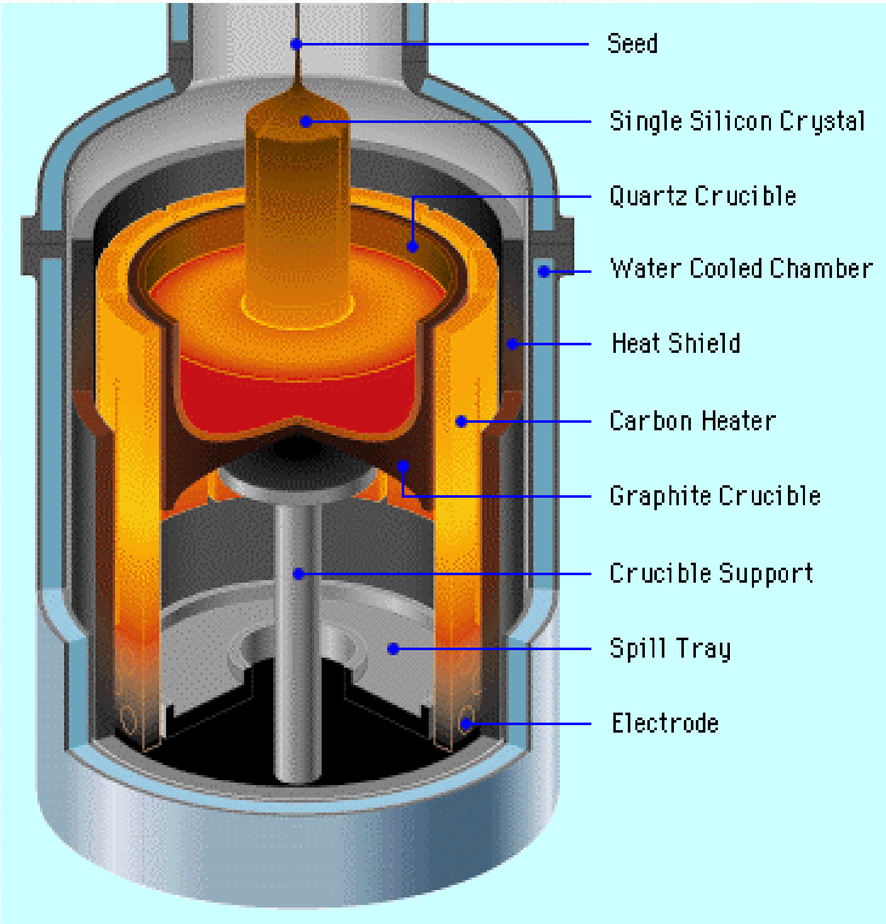
- Associated numberical features
  - Steady-state, transient
  - Stabilization
  - ALE formulation
- Typical couplings
  - FSI
  - Thermal flows (natural convection)
  - Transport
  - Free surface
  - Particle tracker
- Known limitations
  - Only experimental segregated solvers
  - Stronger in the elliptic regime of N-S i.e. low Re numbers
  - RANS models have often convergence issues

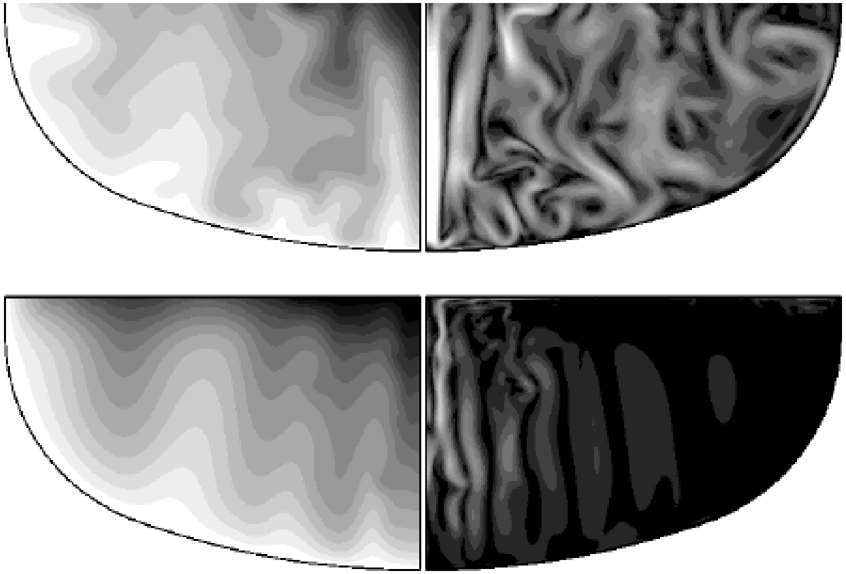
Czockralski Crystal Growth

- 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.



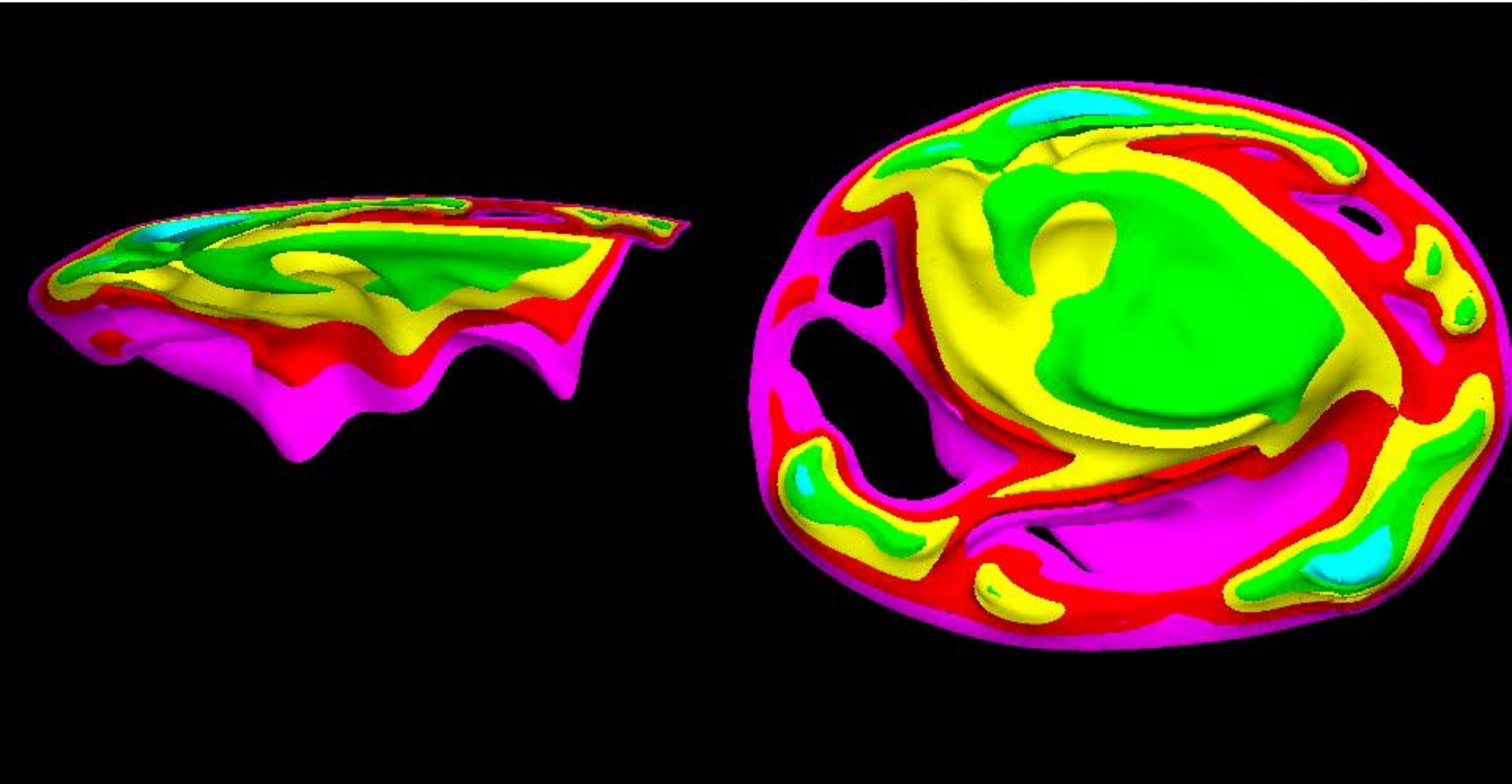


V. Savolainen et al., *Simulation of large-scale silicon melt flow in magnetic Czochralski growth*, J. Crystal Growth 243 (2002), 243-260.

CZ-growth: Transient simulation

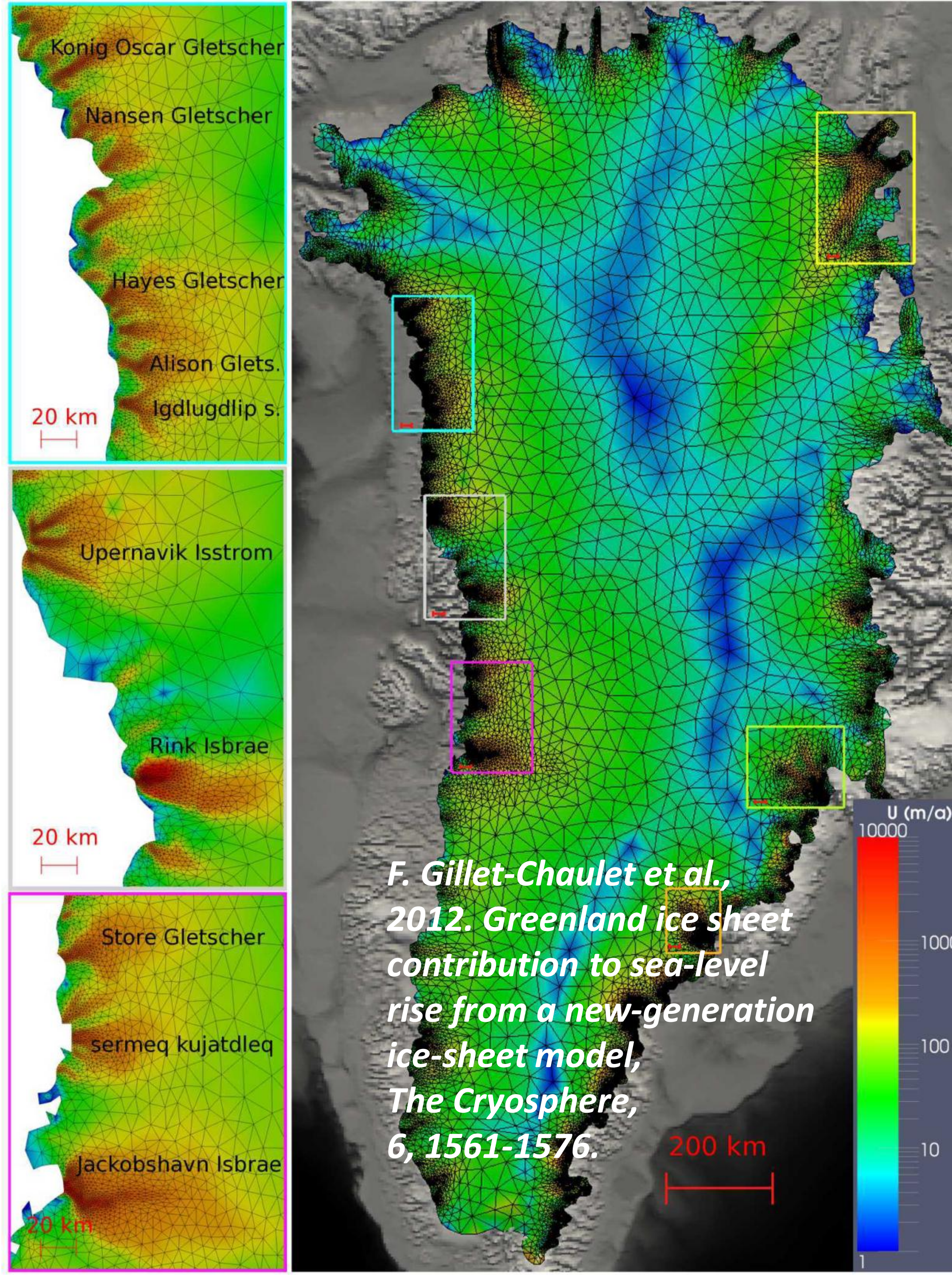
Parallel simulation of silicon meltflows using stabilized finite element method (5.4 million elements).

Simulation Juha Ruokolainen, animation Matti Gröhn, CSC



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

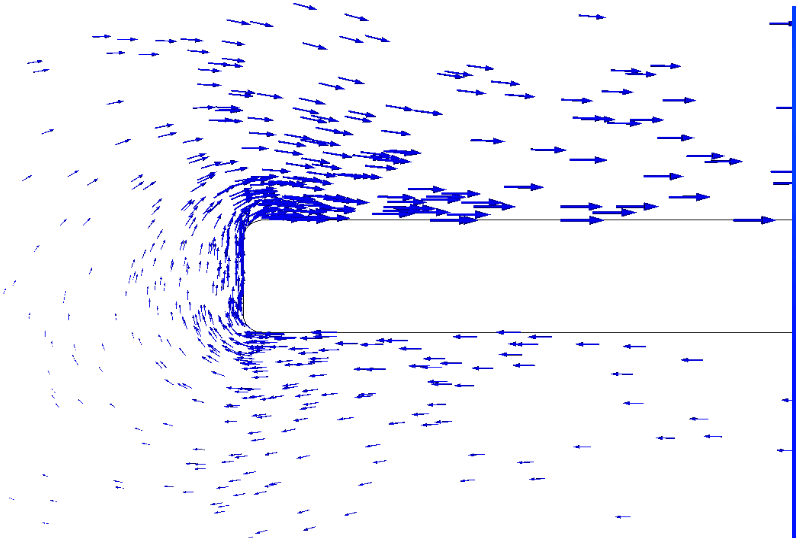
2D compressible Navier-Stokes eq. with heat eq. plus two rarefied gas effects:

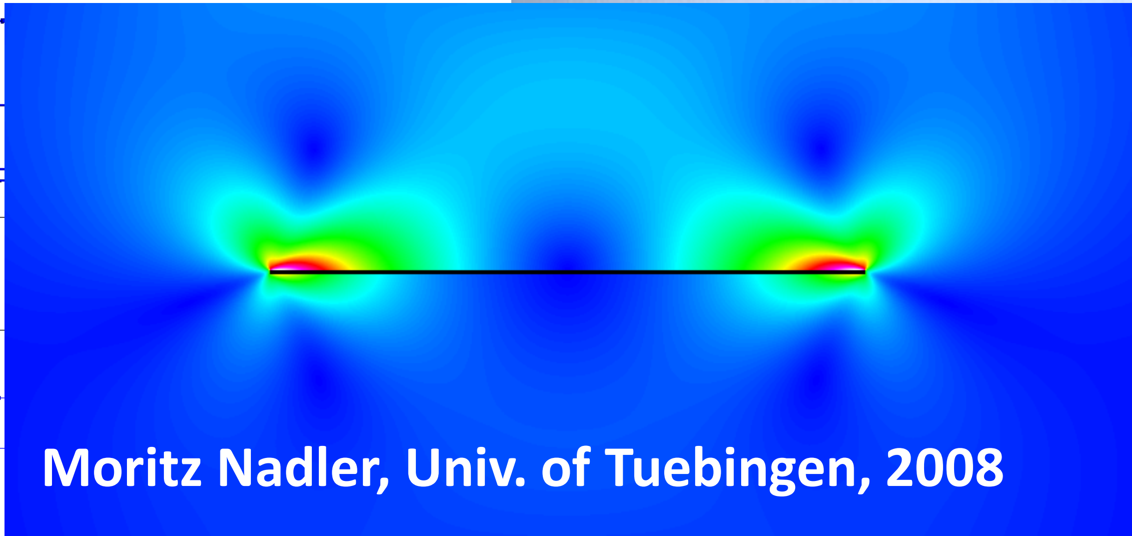
- Maxwell's wall slip and thermal transpiration

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

- Smoluchowski's temperature jump

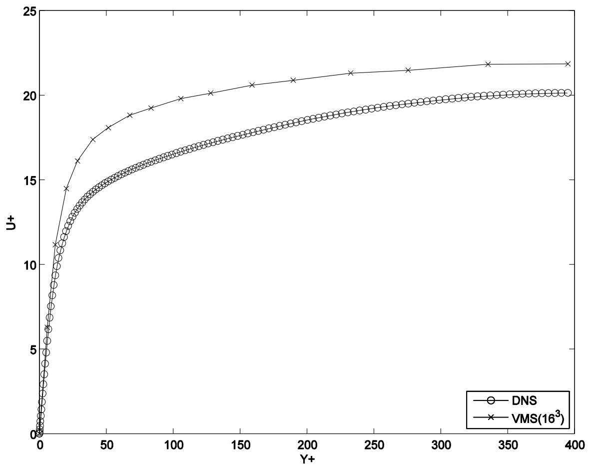
$$T_G - T_W = \frac{2-\sigma_T}{\sigma_T}\frac{2\gamma}{\gamma+1}\frac{\lambda}{Pr}\frac{\partial T}{\partial n}$$



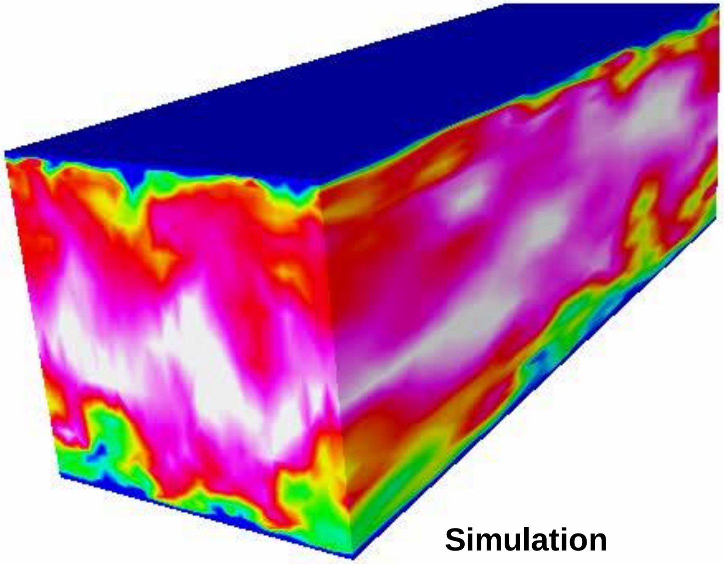


VMS turbulence modeling

- 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

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

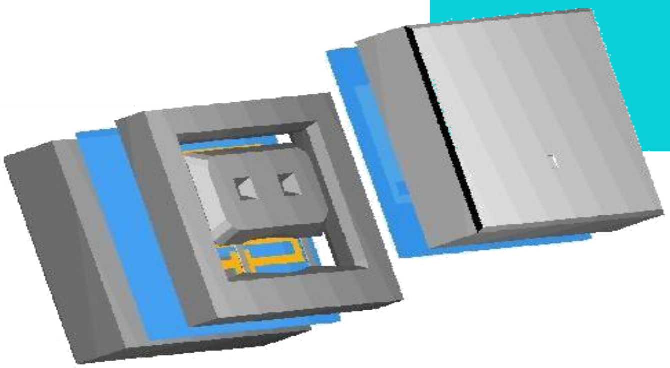
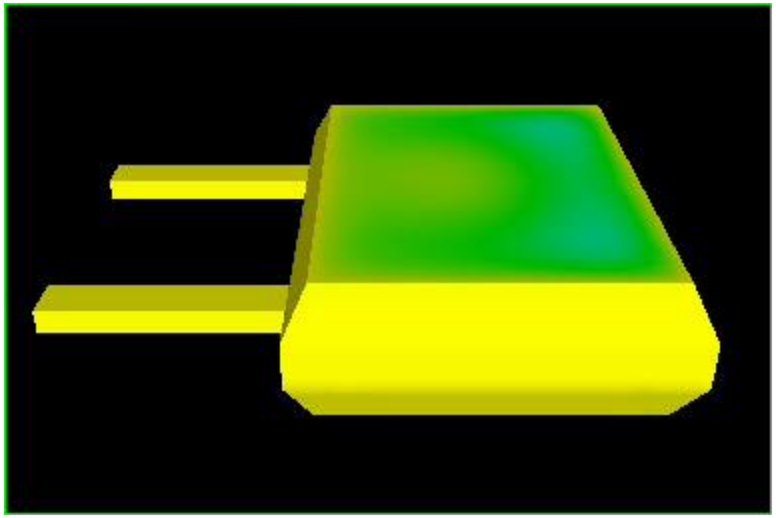
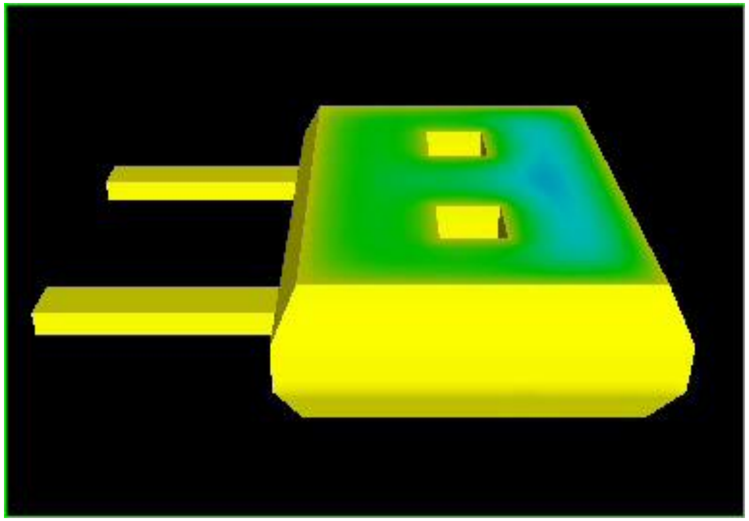


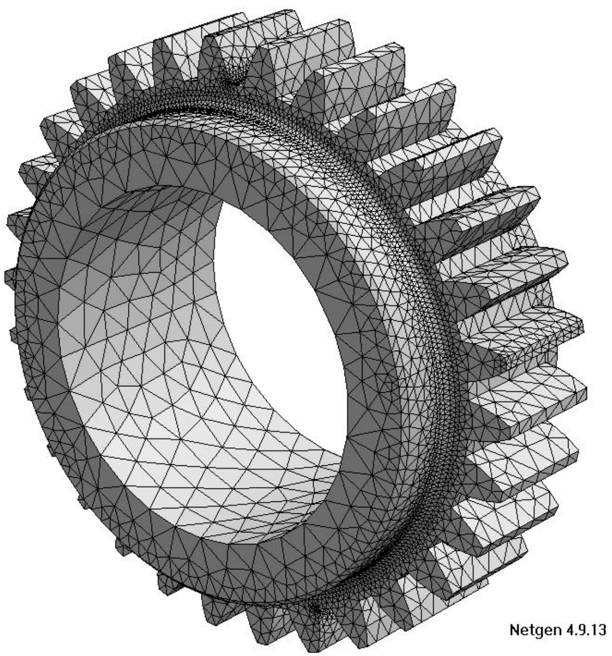
Figure by VTI Technologies

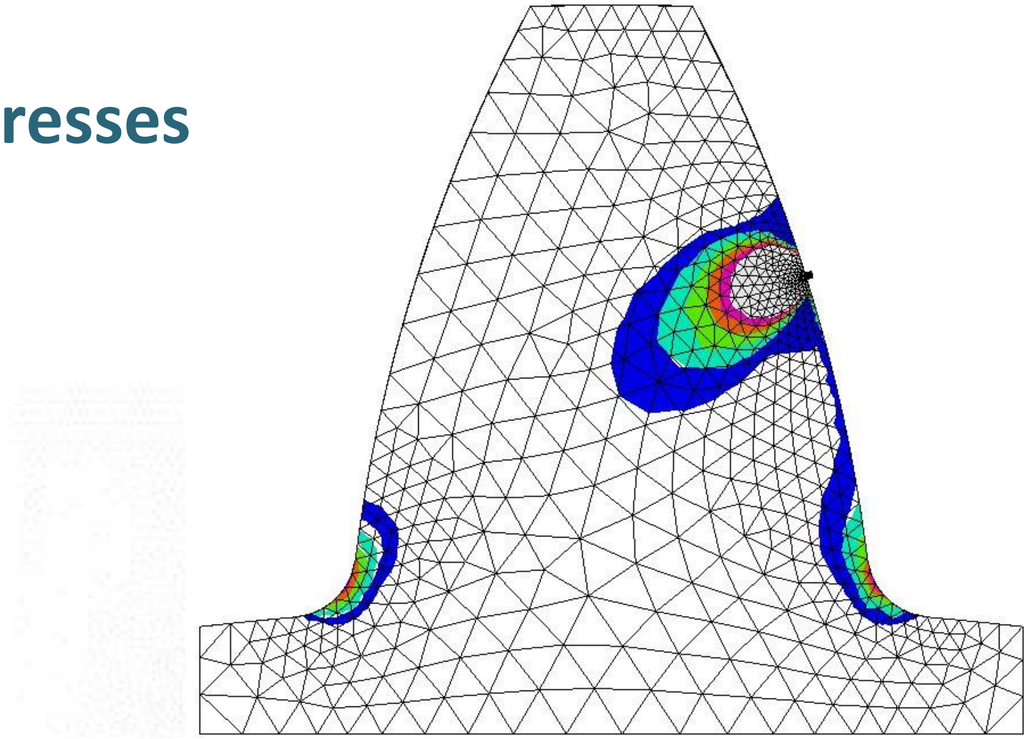


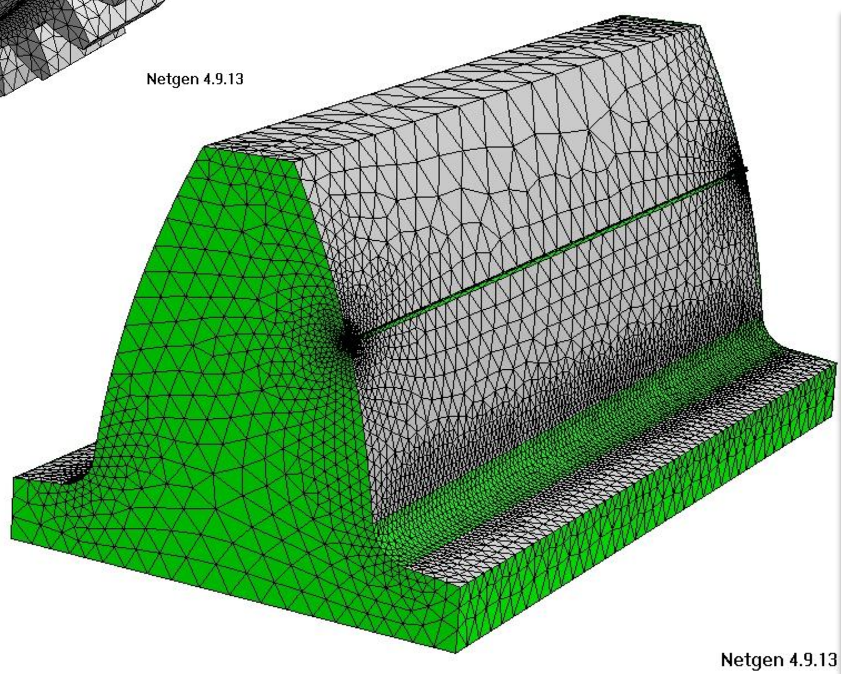


A. Pursula, P. Råback, S. Lähteenmäki and J. Lahdenperä, *Coupled FEM simulations of accelerometers including nonlinear gas damping with comparison to measurements*,
J. Micromech. Microeng. **16** (2006), 2345-2354.

Elasticity – von Mises stresses





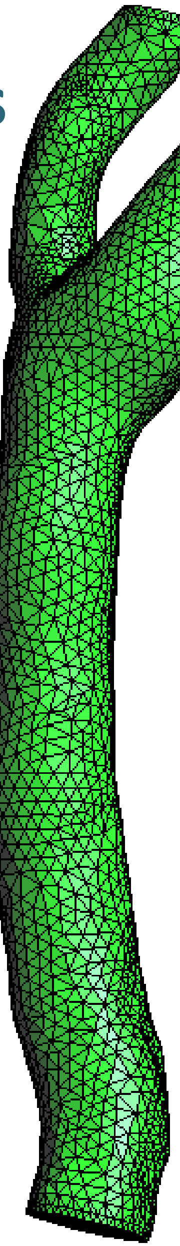


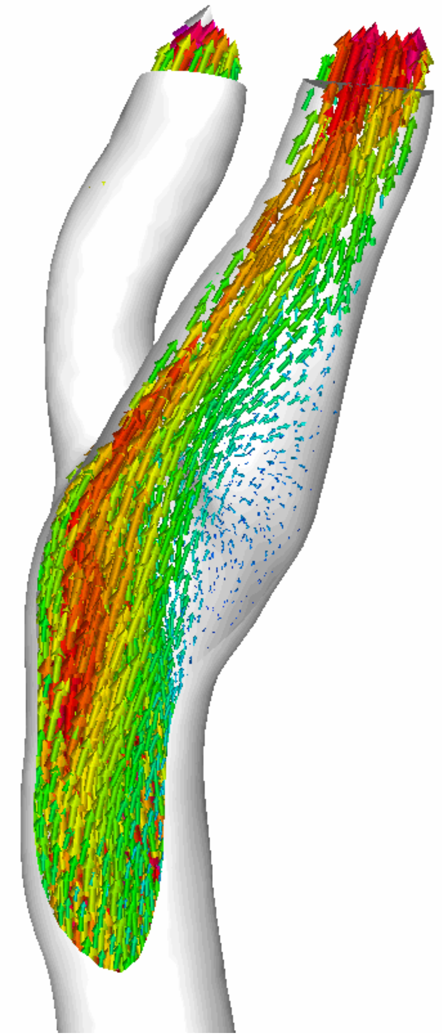
STUDIO D'INGEGNERIA
GARATTONI
progettazione meccanica

http://www.studiogarattoni.com/

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

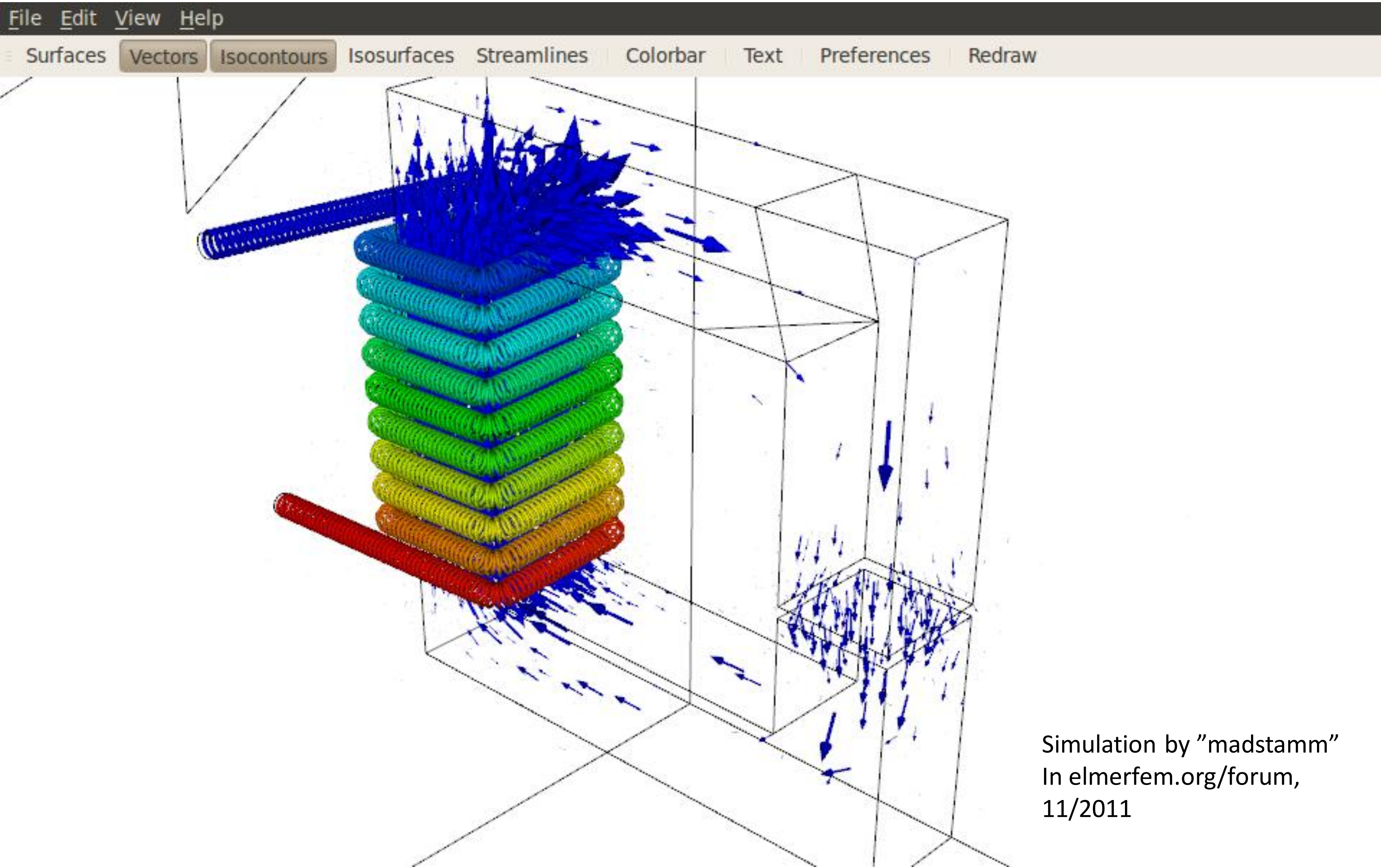
E. Järvinen, P. Råback, M. Lyly, J. Salonius. *A method for partitioned fluid-structure interaction computation of flow in arteries. Medical Eng. & Physics*, **30** (2008), 917-923

Elmer – 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

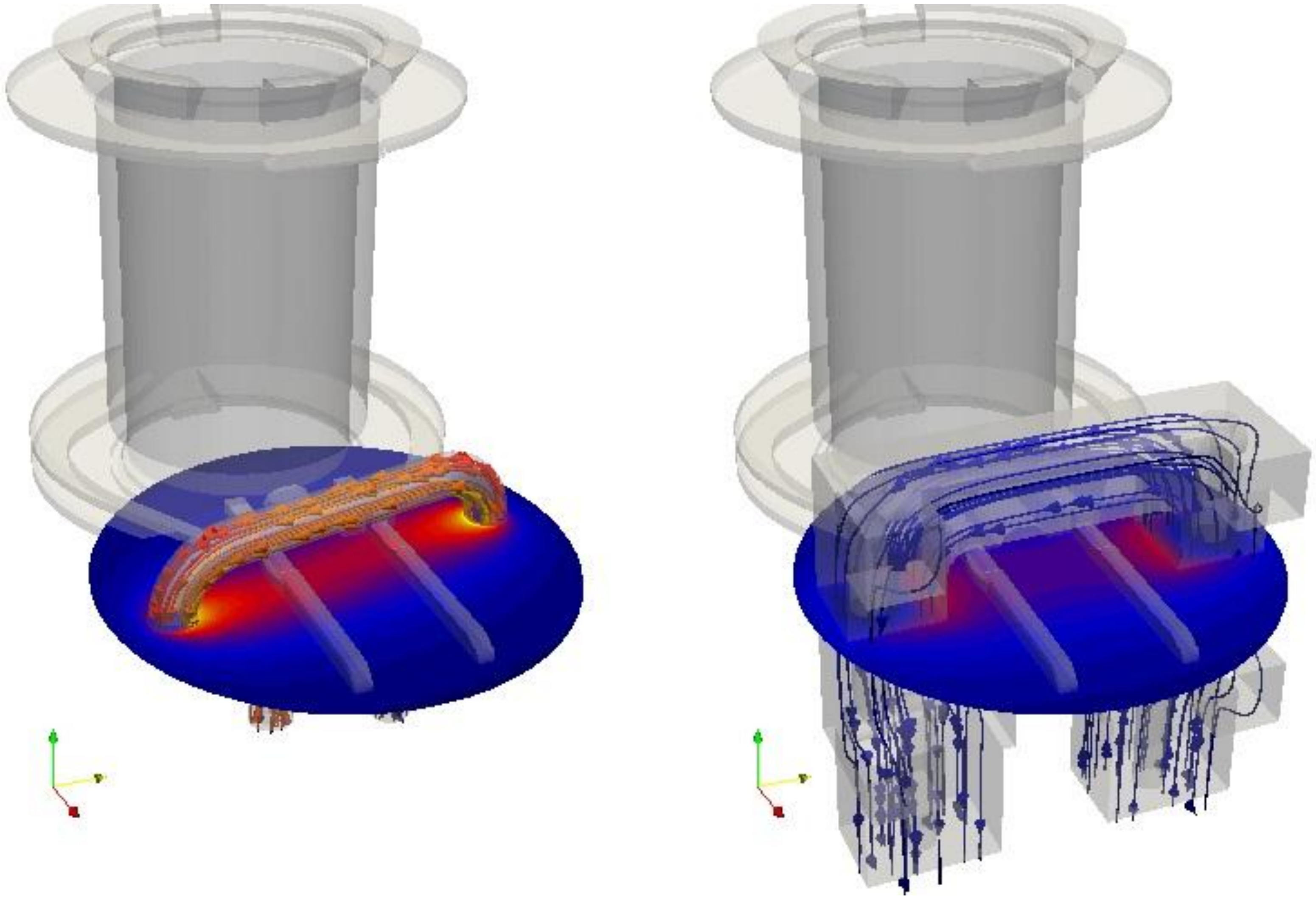
- Associated numerical features
  - Mainly formulations based on scalar and vector potential
  - Lagrange elements except mixed nodal-edge elements for AV solver
- Typical physical couplings
  - Thermal (Joule heating)
  - Flow (plasma)
  - Rigid body motion
- Known limitations
  - Limited to low-frequency (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

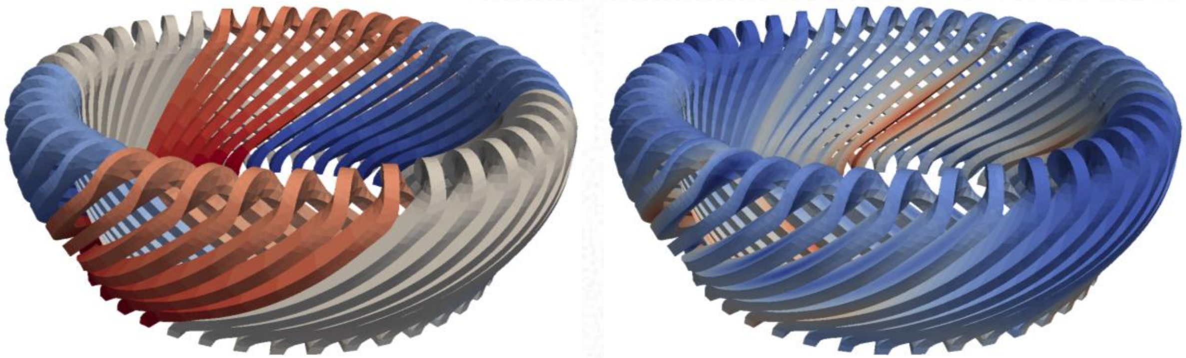
Simulation of Welding



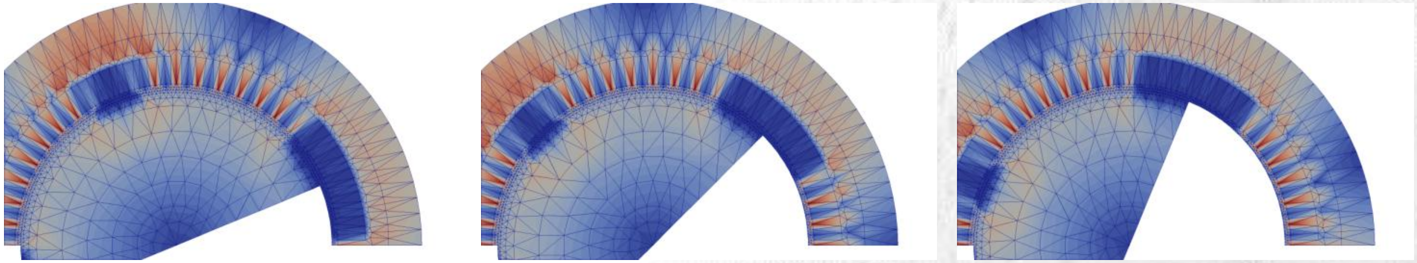
Simulation by Alessandro Rovera, Bitron, Italy, 2014.

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.



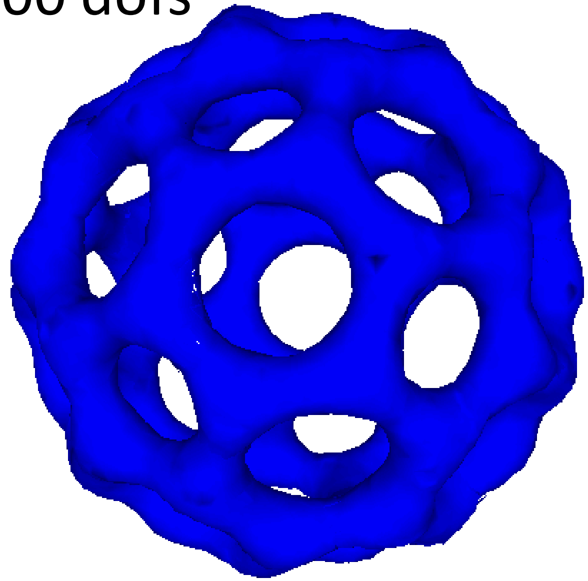
Model specification Antero Arkkio, Meshing Paavo Rasilo, Aalto Univ. Simulation Juha Ruokolainen, CSC, 2013.

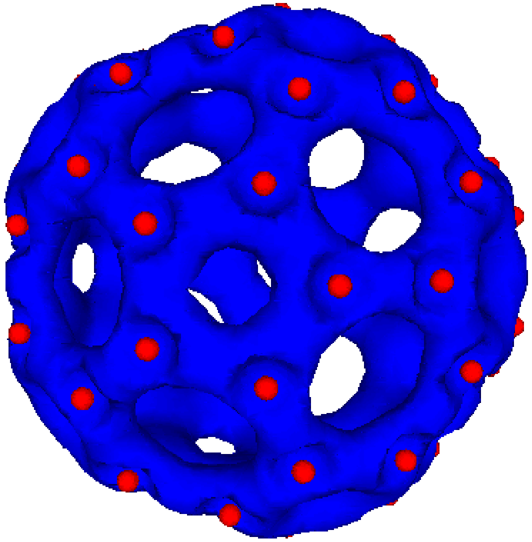
Elmer – other physical models

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

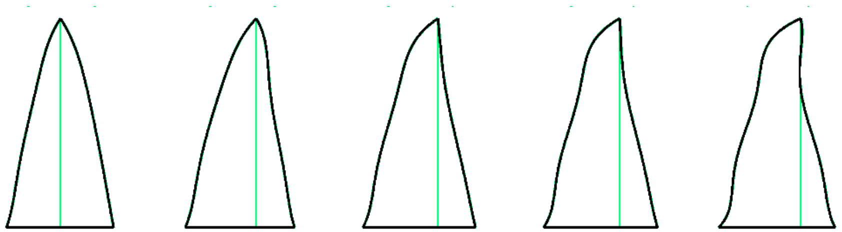




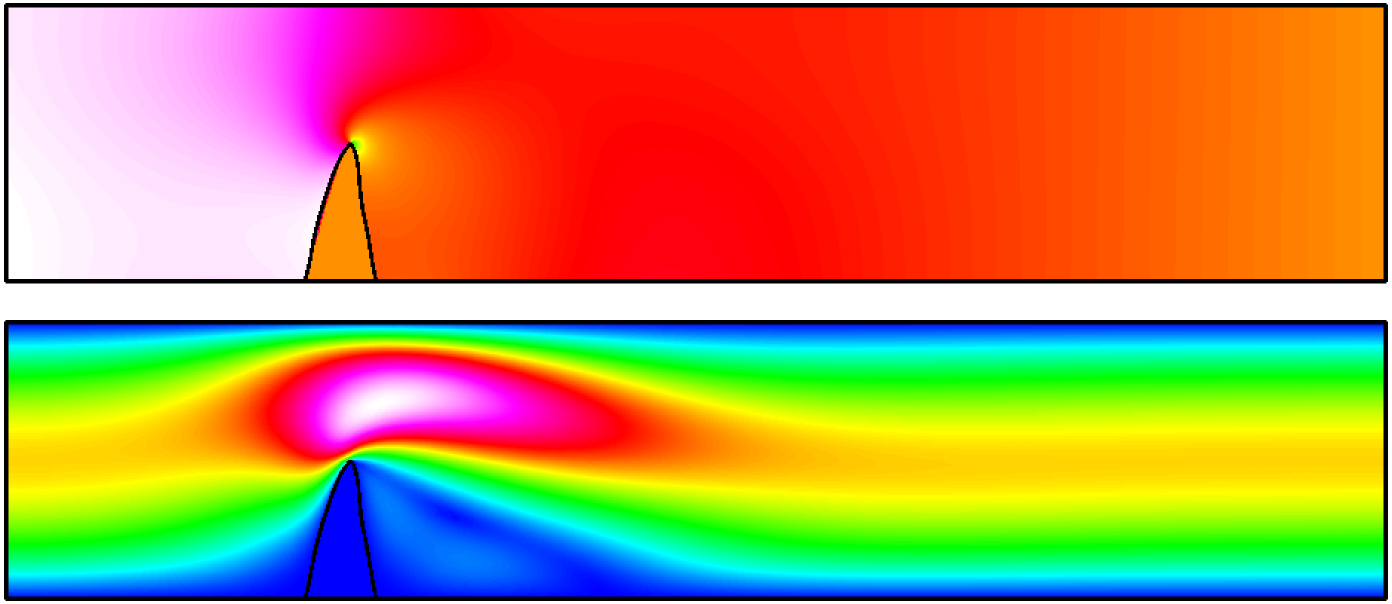
Simulation Mikko Lyly, CSC, 2006

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



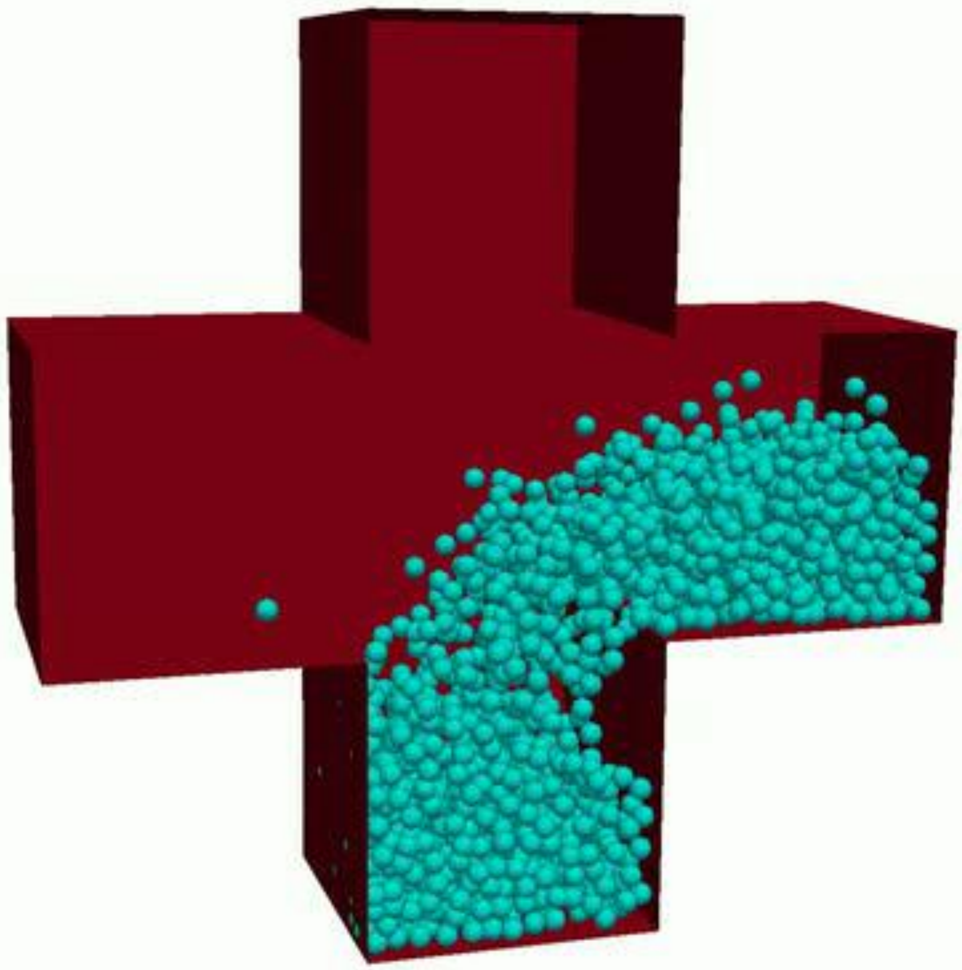
Optimized profiles for Re={0,10,50,100,200}



Pressure and velocity distribution with Re=10

Simulation Peter Råback, CSC

Particle tracker - Granular flow

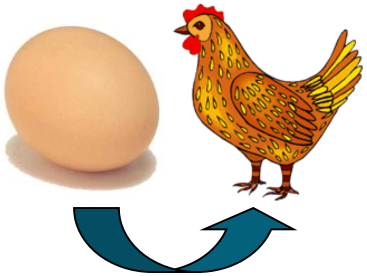


Simulation Peter Råback, CSC, 2011.

Elmer – Selected multiphysics features

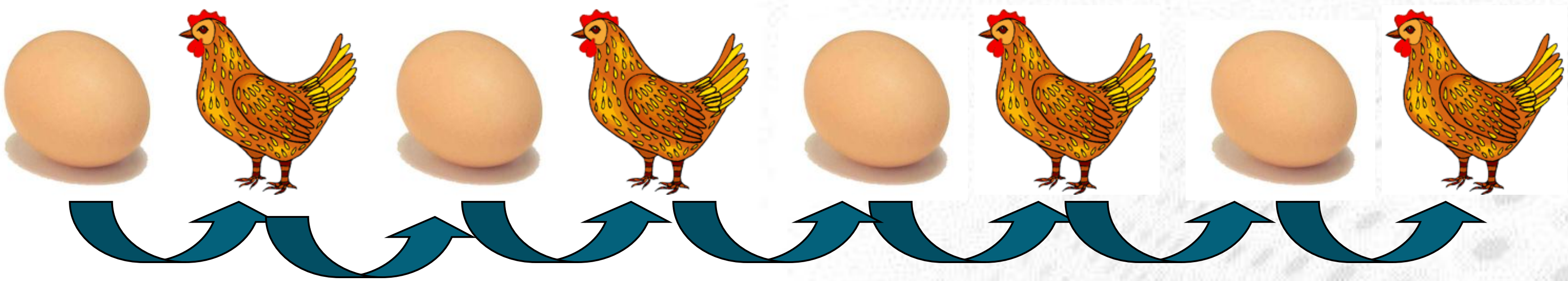
- Solver is an asbtract dynamically loaded object
  - Solver may be developed and compiled without touching the main library
  - No upper limit to the number of Solvers (Currently ~50)
- Solvers may be active in different domains, and even meshes
  - Automatic mapping of field values
- Parameters of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

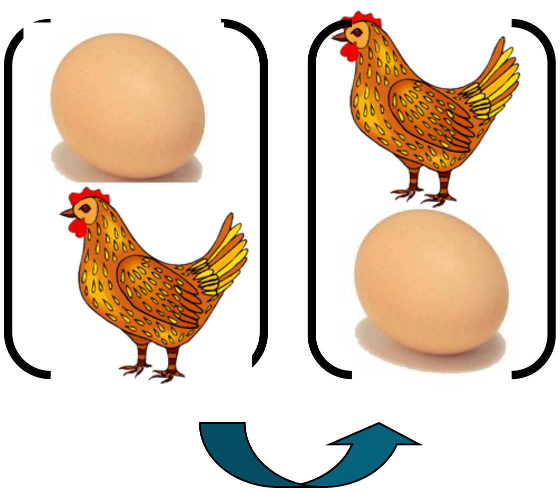
Solution strategies for coupled problems



Hierarchical solution

Iterative solution



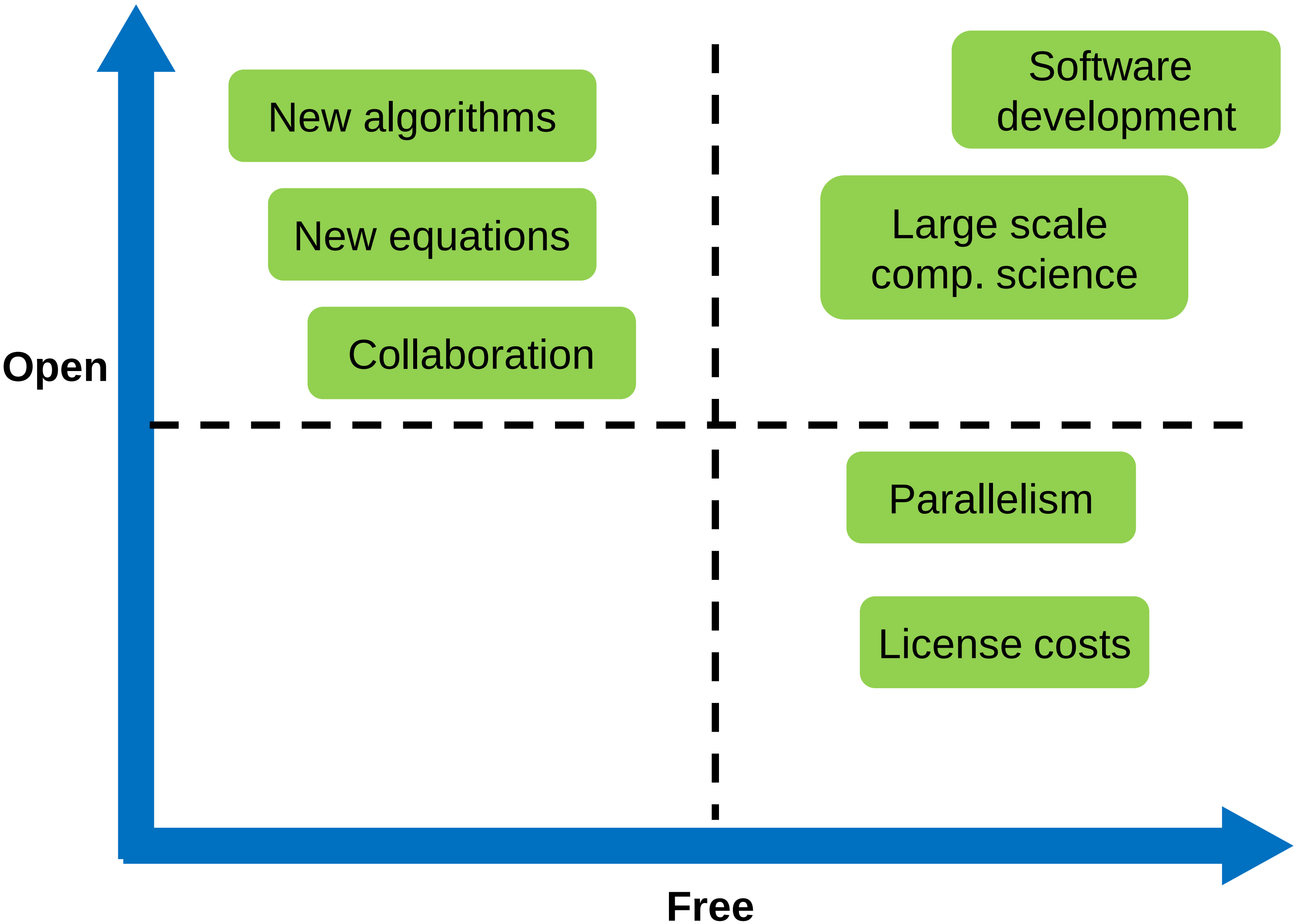


Monolithic solution

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"



Savings from license costs

- A common motivation for using OS software
  - As the only reason may result to disapoinment
- 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 commerial software
  - Excellent libraries for software development (Qt, python,...)

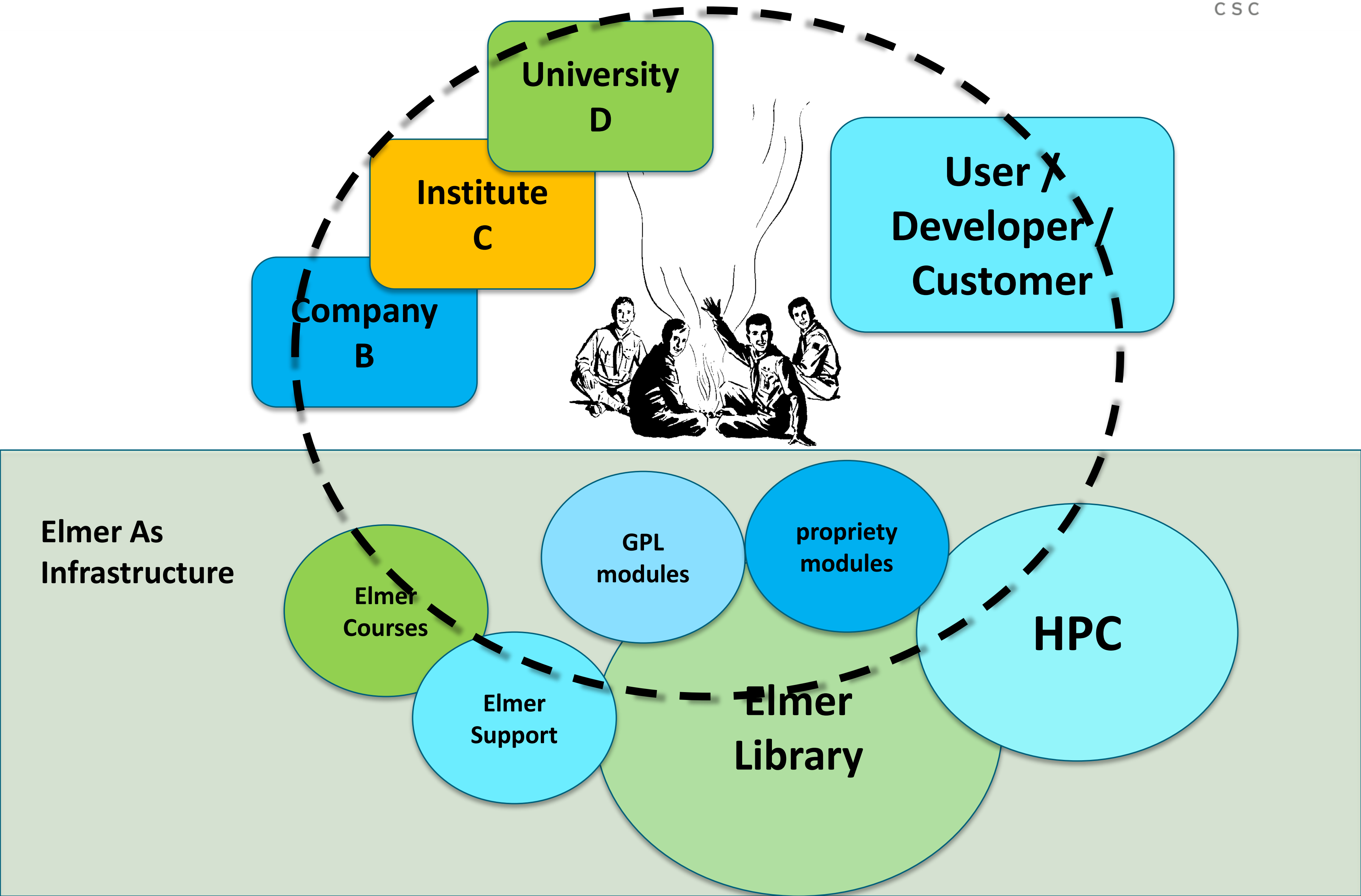
Weaknesses of OS software in CE

- 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 hich-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



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!