Elmer – Open source finite element software for multiphysical problems

Elmer

Open Source Finite Element Software for Multiphysical Problems

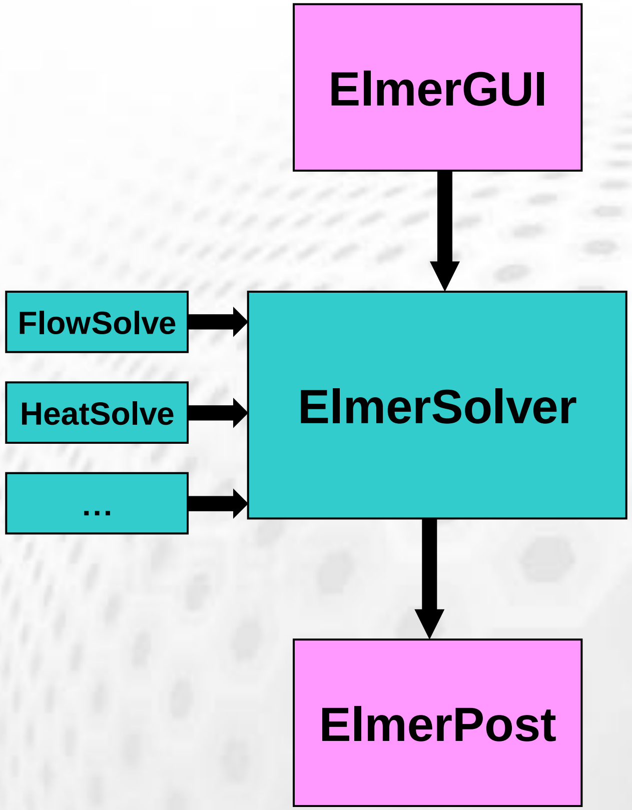
ElmerTeam

CSC – IT Center for Science Ltd.

Elmer Course
CSC, 9-10.1.2012

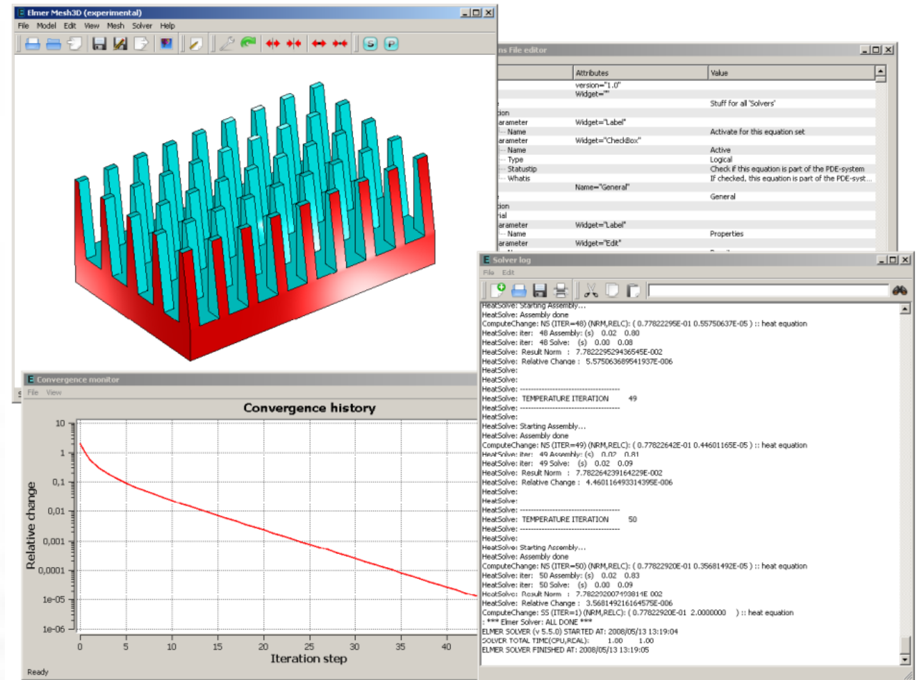
Components of Elmer software suite

- Elmer is actually a suite of several programs
- You may use many of the components independently
- ElmerGUI – Pre- and Postprocessing
- ElmerSolver - Solution
- ElmerPost - Postprocessing
- ElmerGrid – structured meshing and mesh import
- Others
  - ElmerFront: the old preprocessor
  - Mesh2D: Delaunay mesher usable through ElmerFront
  - MATC: library for on-the-fly arithmetics
  - ElmerParam: black-box interfacing of ascii-file based simulations



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



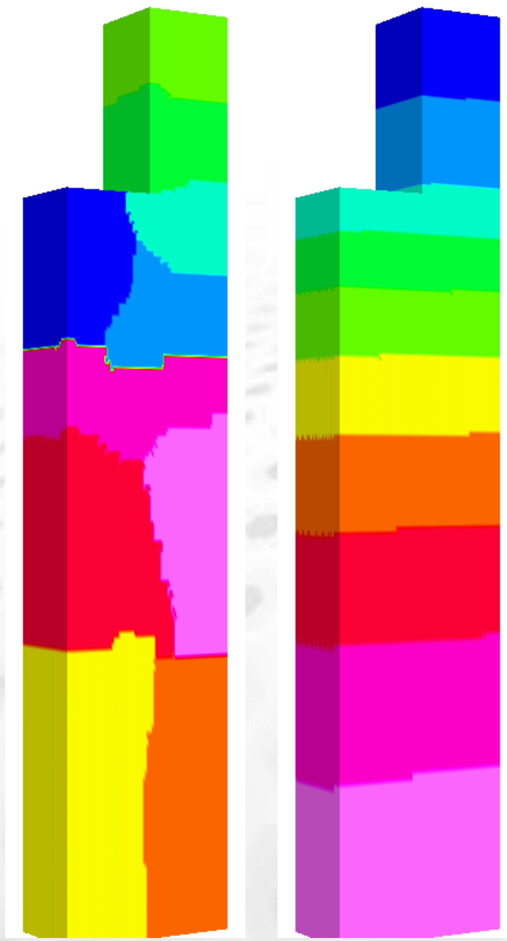
ElmerSolver

- Assembly and solution of the finite element equations
- Parallelization by MPI
- 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
```

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,…)



Elmer – Numerical Methods

- Time-dependency
  - Static, transient, eigenmode, scanning
- Discretization
  - Galerkin, Discontinous Galerkin (DG)
  - Stabilization, Bubbles
  - Lagrange, edge, face, and p-elements
- Matrix equation 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,…
- Parallellism
  - Parallel assembly and solution (vector-matrix product)
- Adaptivity
  - For selected equations, works well in 2D

Elmer - Physical Models

- Heat transfer
  - Heat equation
  - Radiation with view factors
  - convection and phase change
- Fluid mechanics
  - Navies-Stokes (2D & 3D)
  - Turbulence models: k-ε, v^2-f, *VMS*
  - Reynolds (2D)
- Structural mechanics
  - Elasticity (unisotropic, lin & nonlin)
  - Plate, Shell
- Free surface problems
  - Lagrangian techniques
  - Level set method (2D)
- Mesh movement
  - Extending displacements in coupled problems
  - ALE formulation
- Acoustics
  - Helmholtz
  - Linearized time-harmonic N-S
- Species transport
  - Generic convection-diffusion equation
- Electromagnetics
  - Emphasis on steady-state and harmonic analysis
  - New Whitney element formulation for magnetic fields
- Electrokinetics
  - Poisson-Boltzmann
  - Poisson-Nernst-Planck
- Quantum mechanics
  - DFT (Kohn Scham)
- Particle Tracker
- ….

Application Fields – Poll (Jan 2012)

What are your main application fields of Elmer?

You may select up to **5** options

Heat transfer	☑	49	**30%**
Fluid mechanics	☑	48	**29%**
Solid mechanics	☑	36	**22%**
Electromagnetics	☐	22	13%
Quantum mechanics	☐	3	2%
Something else (please specify)	☐	6	4%

Total votes : 164

Submit vote

Elmer - Multiphysics capabilities

- About 20 different physical models
- Iteration method is mainly used
  - Consistancy of solution is ensured by nested iterations
- Monolithic approach is used for some inherently coupled problems
  - Linearized time-harmonic Navier-Stokes
  - Recently new generic strategies have been implemented for monolithic problems
- For some special problems using iterative coupling convergence has been improved by consistant manipulation of the equations
  - Fluid-structure interaction
  - Pull-in analysis
- High level of abstraction ensures flexibility in implementation and simulation
  - Each model is an external module with standard interfaces to the main program
  - All models may basically be coupled in any way
  - Different models may occupy different computational domains
  - Different models may use different meshes and the results are mapped between them

Nature of coupling

- The mathematical analysis does not give strict guidelines for the solution methods of coupled problems
  - Even uniqueness of solution is difficult to show
  - Heuristic approach: if the method works, use it
- Computational cost of coupled problems is often significantly larger than the combined solution time of individual probelms
- The strength of coupling of individual phenomena is reflected in the difficulty of solution
  - One-directional coupling -> hierarchical solution
  - Weak coupling easy -> iterative solution
  - Strong coupling difficult -> monolithic solution

Solution strategies for coupled problems

Assume phenomena $\mathcal{F}$ and $\mathcal{G}$ that both depend on field variables x and y.
Solution is obtained from a system of equations, $f(x, y) = 0$ and $g(y, x) = 0$.

one-directional coupling $\Rightarrow$ hierarchical solution

$$\begin{aligned} & f(x_1) &= 0 \\ \Rightarrow \quad & g(y_1, x_1) &= 0 \end{aligned}$$

weak coupling $\Rightarrow$ iterative or segregated solution

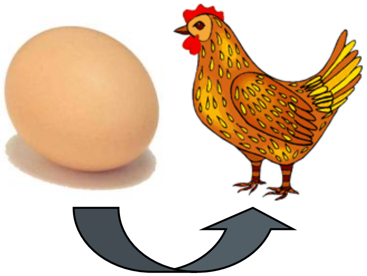
$$\begin{cases} f(x_{m+1}, y_m) &= 0 \\ g(y_{m+1}, x_{m+1}) &= 0 \end{cases}$$

strong coupling $\Rightarrow$ monolithic solution

$$\left[\begin{array}{c} f(x_{m+1}, y_{m+1}) \\ g(y_{m+1}, x_{m+1}) \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \end{array} \right]$$

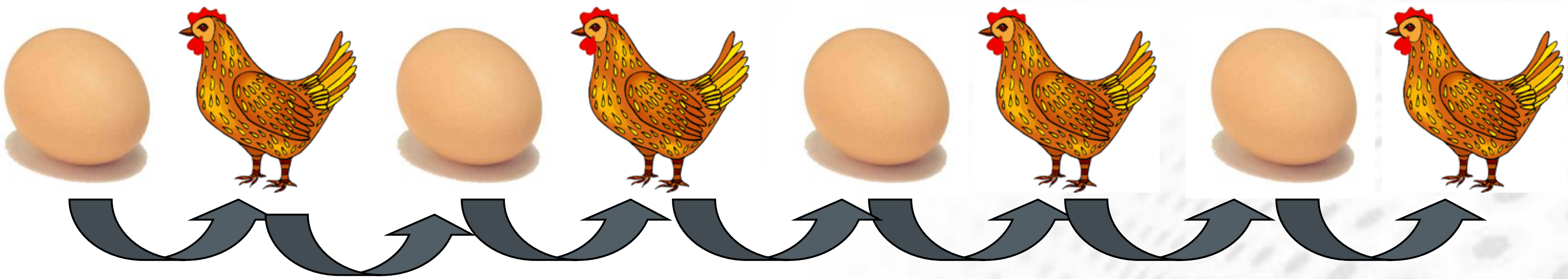
Monolithic approach requires iteration if either f or g is nonlinear.

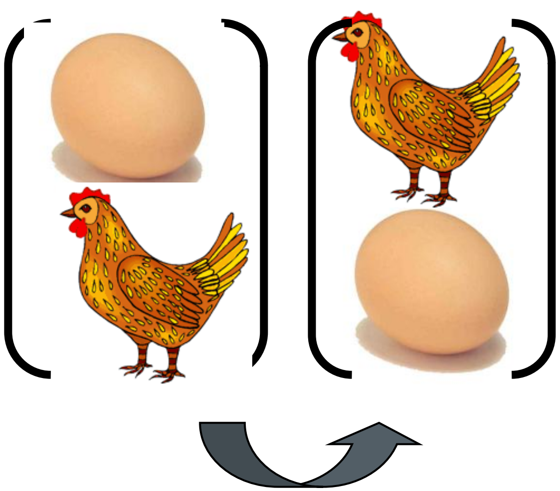
Solution strategies for coupled problems



Hierarchical solution

Iterative solution





Monolithic solution

Short history of Elmer

- 1995 Elmer development was started as part of a national CFD program
  - Collaboration with TKK, VTT, JyU, and Okmetic Ltd.
- 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
  - Roughly 400 000 lines of code
- 2010 Used wordwide by thousands (?) of researchers
  - About 1000 downloads of the Windows binary each month
  - ~50000 visits to community forum from ~120 countries during last year
- Readily available in major Linux systems
- Application projects are nowadays mainly international
  - Used in a number of EU-projects
  - Central tool in computational glaciology

Elmer - Developers

- Current main developers
  - CSC: Mika Malinen, Juha Ruokolainen, Peter Råback, Sampo Sillanpää, Thomas Zwinger
- 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, Mikko Byckling
  - Trueflaw: Iikka Virkkunen
  - Open Innovation: Adam Powell
  - LGGE: Olivier Gagliardini
  - etc…

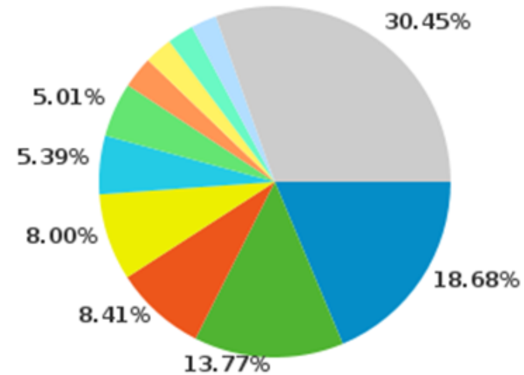
elmerfem.org statistics for 2011: countries

Visits	Pages/Visit	Avg. Time on Site	% New Visits	Bounce Rate
68,784	**4.47**	**00:04:57**	**46.89%**	**51.80%**
% of Site Total: **100.00%**	Site Avg: **4.47 (0.00%)**	Site Avg: **00:04:57 (0.00%)**	Site Avg: **46.73% (0.34%)**	Site Avg: **51.80% (0.00%)**

Detail Level: Country/Territory

	Country/Territory	Visits	Visits
1.	United States	**12,847**	18.68%
2.	Germany	**9,473**	13.77%
3.	Finland	**5,787**	8.41%
4.	France	**5,503**	8.00%
5.	United Kingdom	**3,706**	5.39%
6.	Italy	**3,443**	5.01%
7.	Canada	**2,014**	2.93%
8.	India	**1,767**	2.57%
9.	Japan	**1,676**	2.44%
10.	Spain	**1,619**	2.35%
11.	Russia	**1,391**	2.02%
12.	Netherlands	**1,376**	2.00%
13.	Switzerland	**1,321**	1.92%
14.	Poland	**1,216**	1.77%
15.	China	**1,187**	1.73%
16.	Belgium	**958**	1.39%
17.	Sweden	**882**	1.28%
18.	Australia	**775**	1.13%
19.	Czech Republic	**761**	1.11%
20.	Argentina	**664**	0.97%

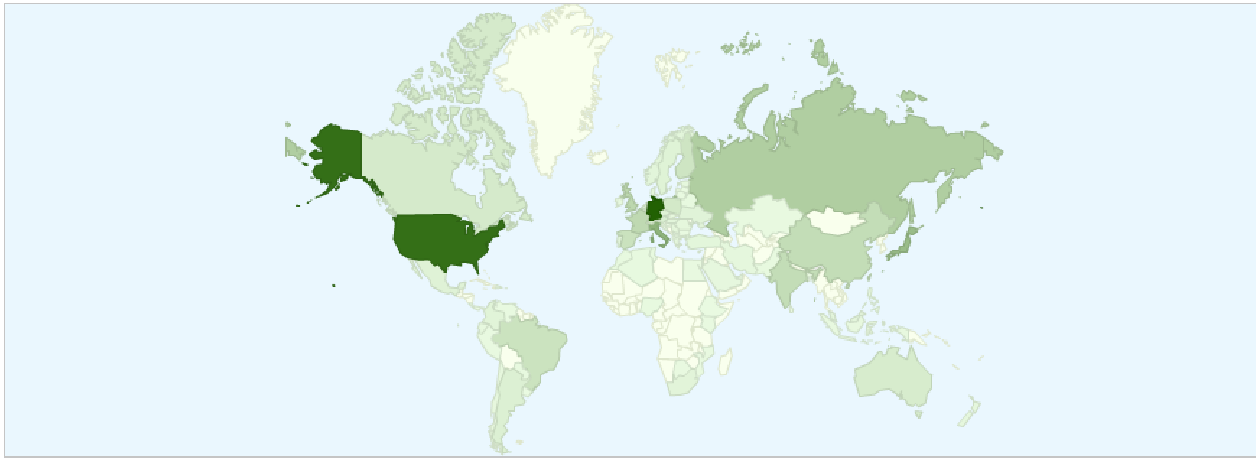
Country/Territory contribution to total: Visits



Elmer windows downloads at sf.net (6 months)

Home / WindowsBinaries (Change File)

Date Range: 2011-05-04 to 2011-11-04



DOWNLOADS

6 837

In the selected date range

TOP COUNTRY

Germany

16% of downloaders

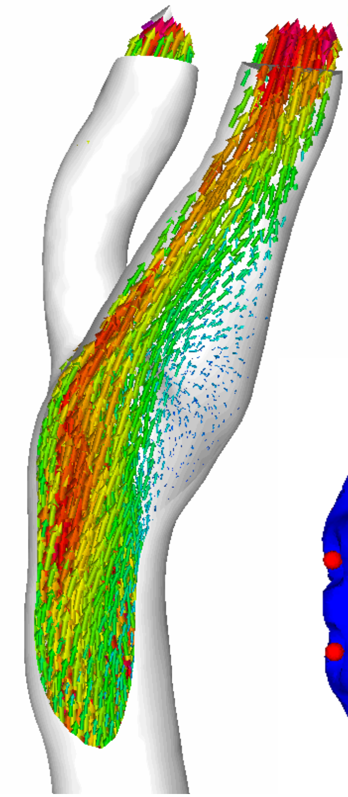
TOP OS

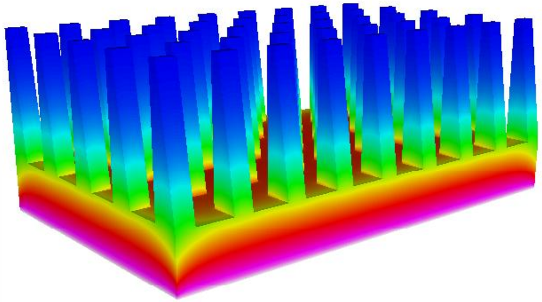
Windows

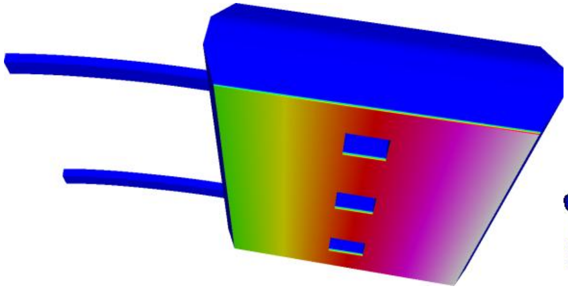
94% of downloaders

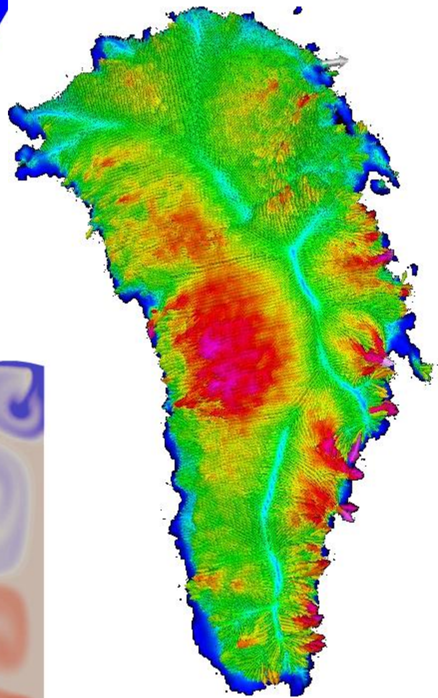
	Country	Downloads
1.	Germany	1,142
2.	United States	1,036
3.	Italy	521
4.	Japan	458
5.	Russia	327
6.	United Kingdom	258
7.	France	241
8.	India	216
9.	China	215
10.	Spain	177

Elmer is also available in several Linux distrbutions beoynd any traffic control

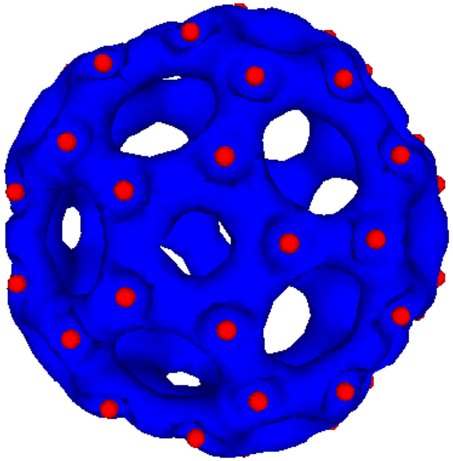


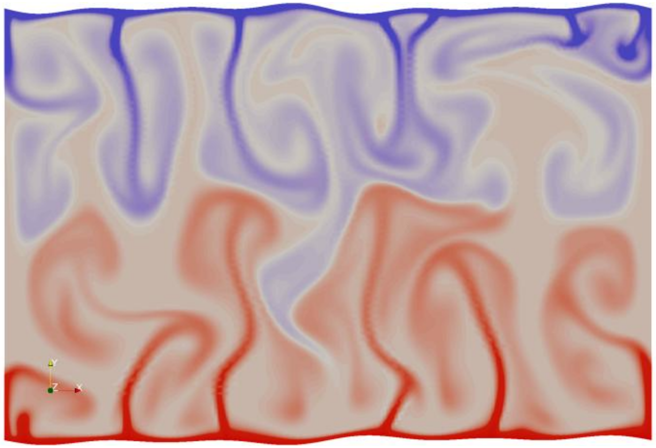


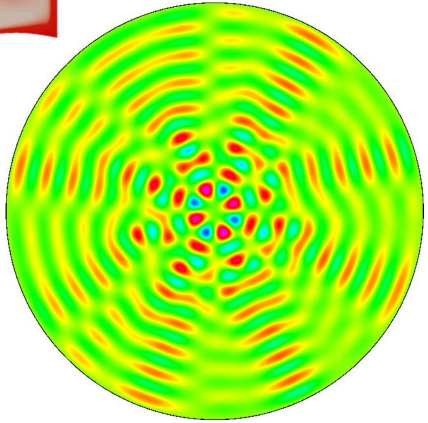


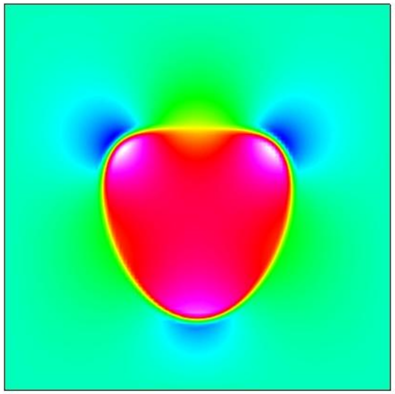


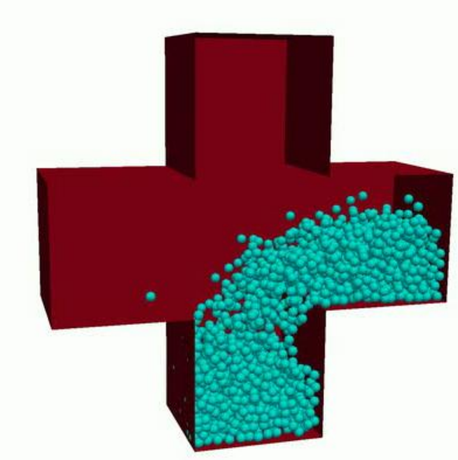
Elmer Simulations

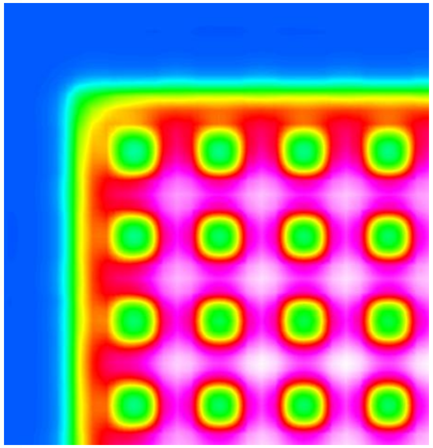








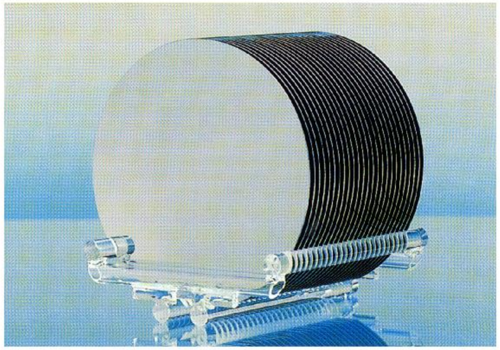




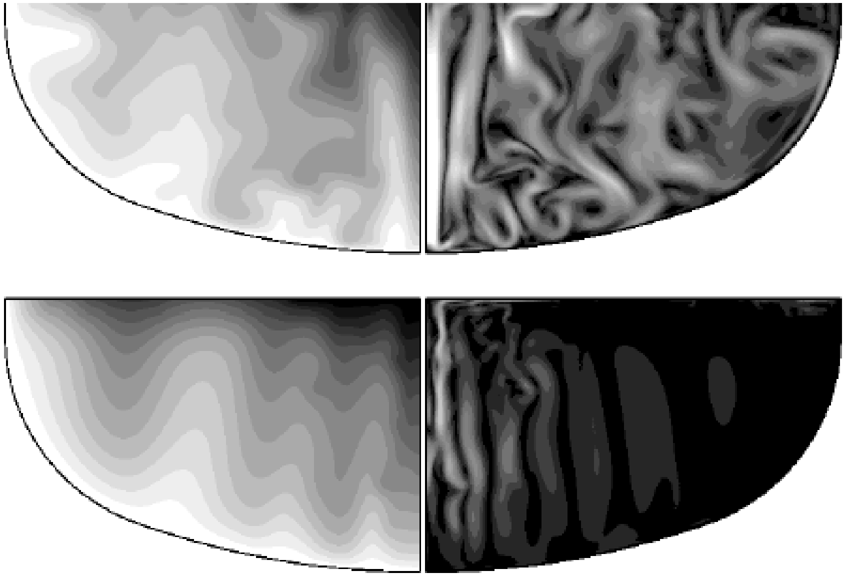
Figures by Esko Järvinen, Mikko Lyly, Peter Råback, Timo Veijola (TKK) & Thomas Zwinger

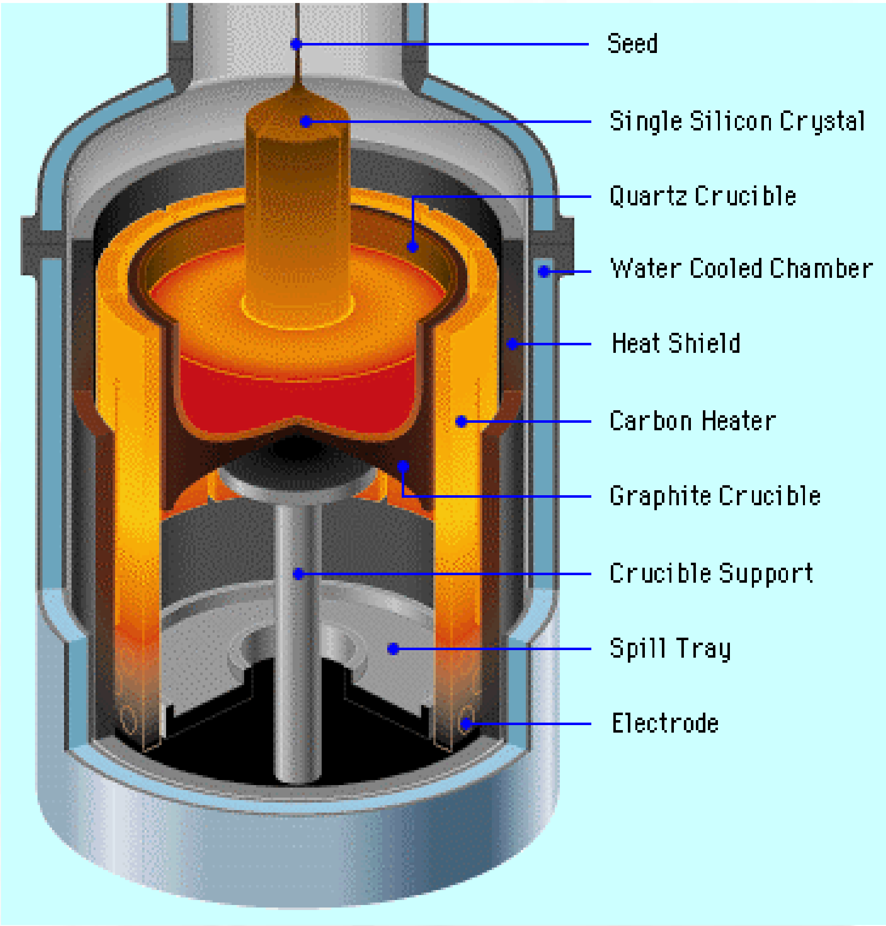
Czockralski Crystal Growth

- 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.



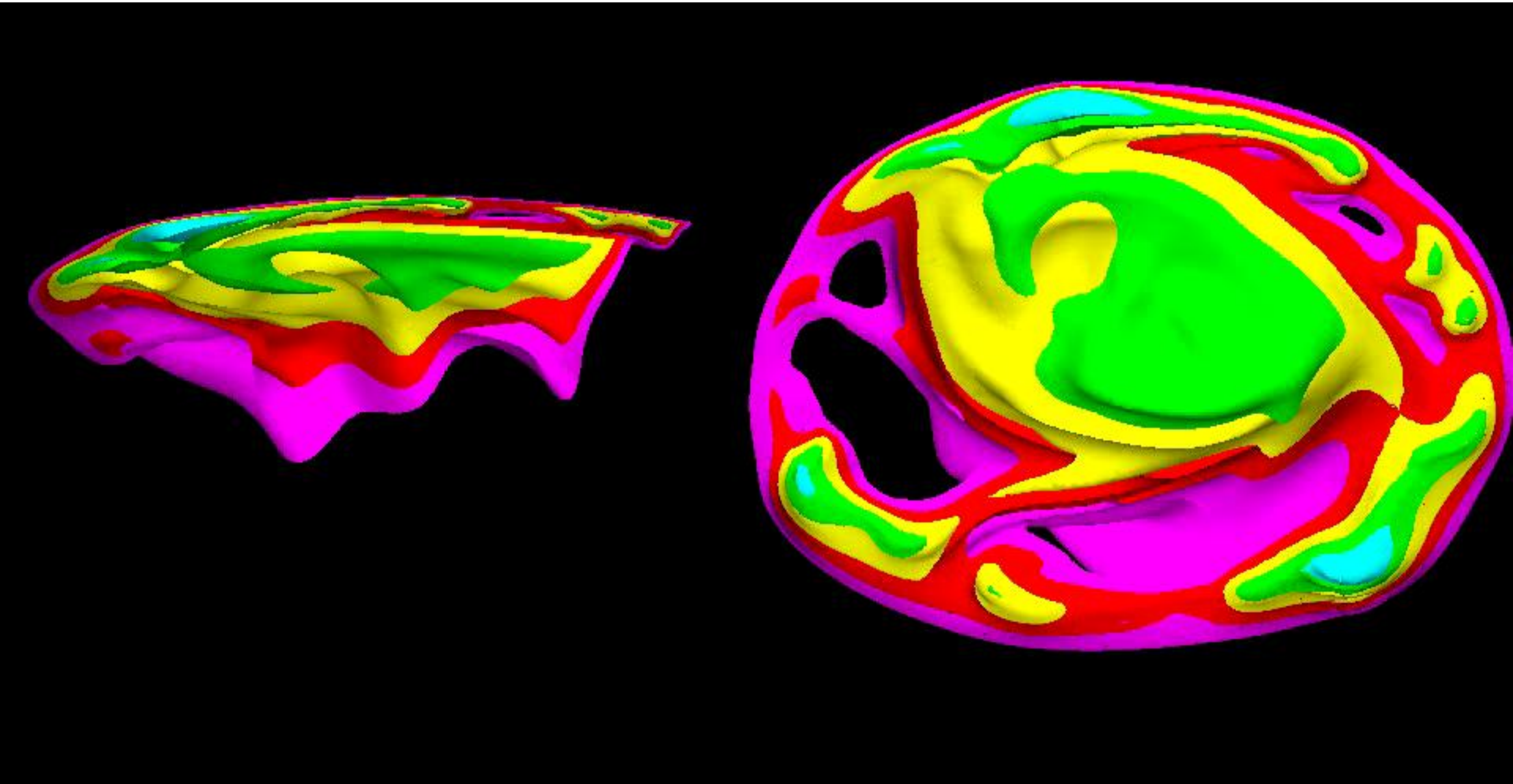


V. Savolainen et al., *Simulation of large-scale silicon melt flow in magnetic Czochralski growth,* J. Crystal Growth 243 (2002), 243-260.

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



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

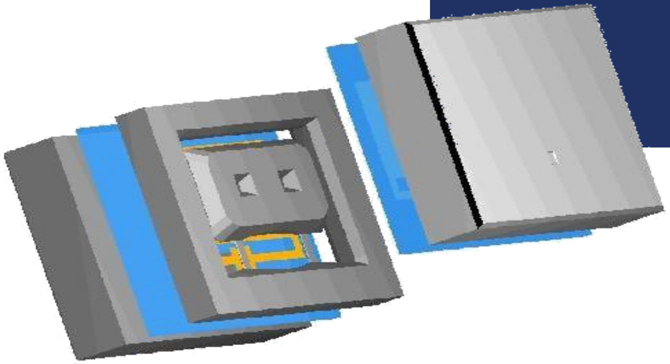
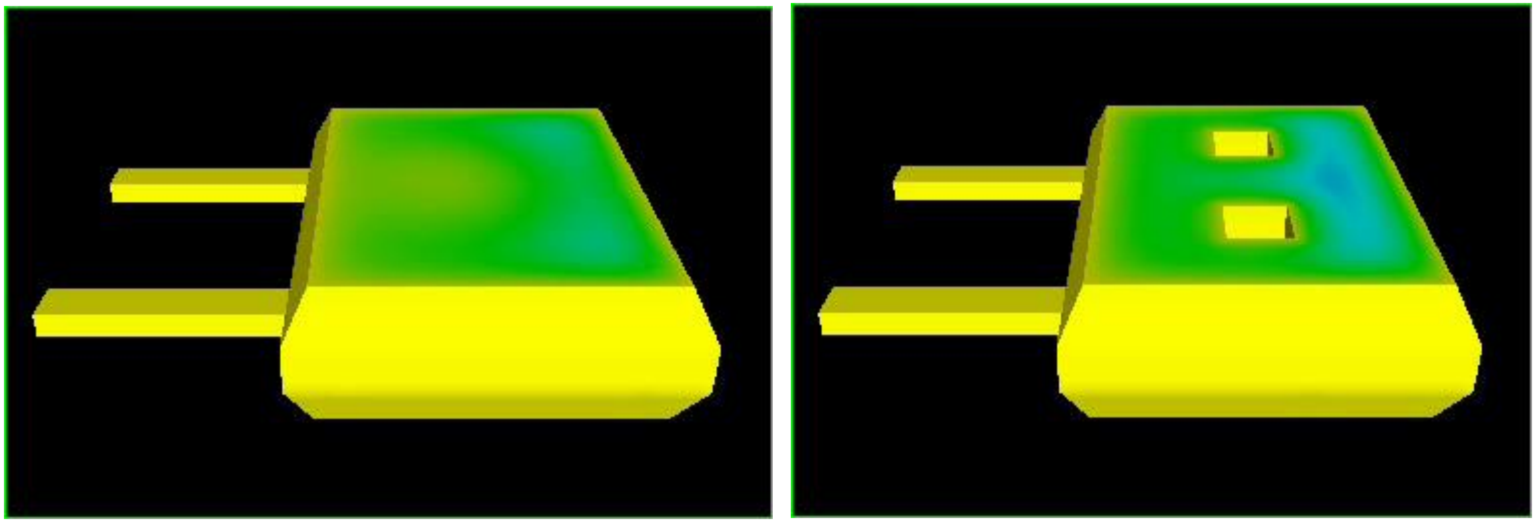
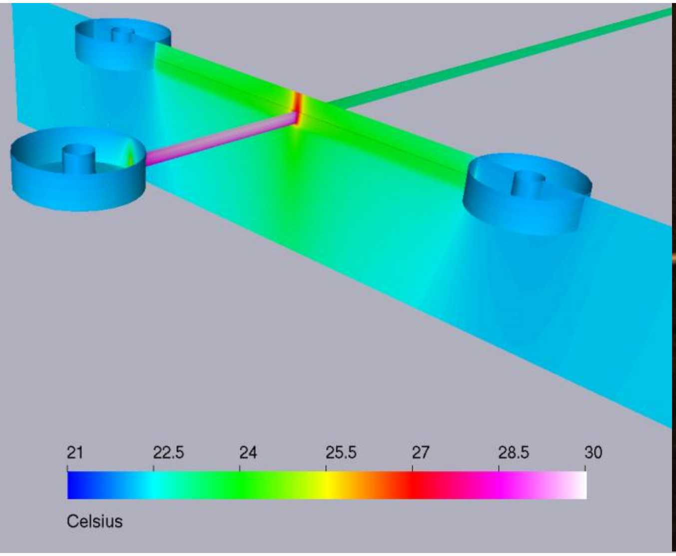


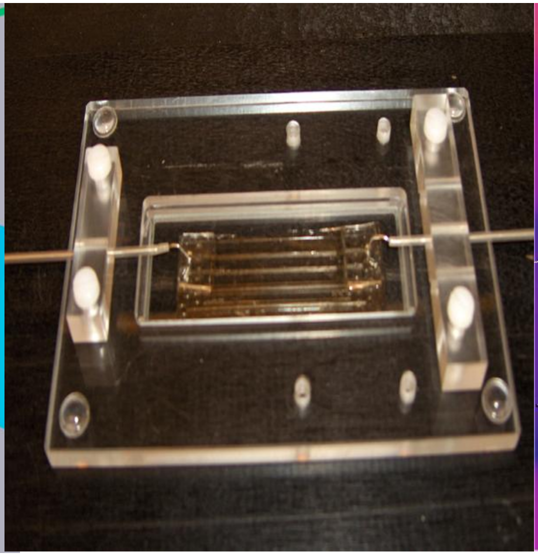
Figure by VTI Technologies

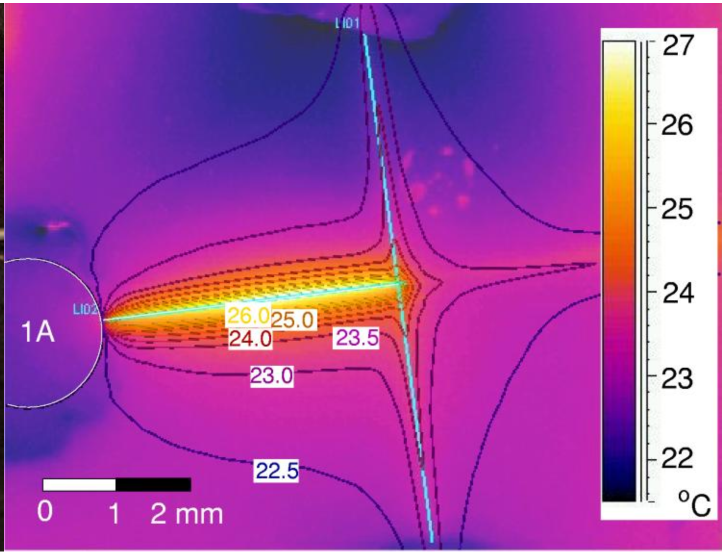


A. Pursula, P. Råback, S. Lähteenmäki and J. Lahdenperä, *Coupled FEM simulations of accelerometers including nonlinear gas damping with comparison to measurements*,
J. Micromech. Microeng. **16** (2006), 2345-2354.

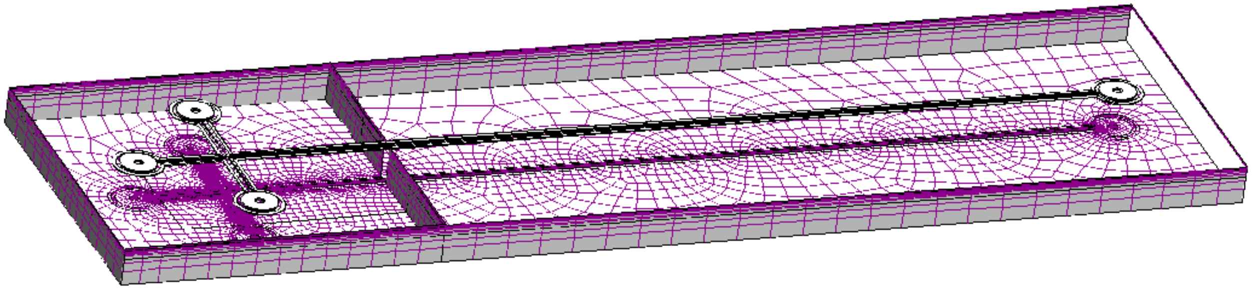
Microfluidics: Flow and heat transfer in a microchip







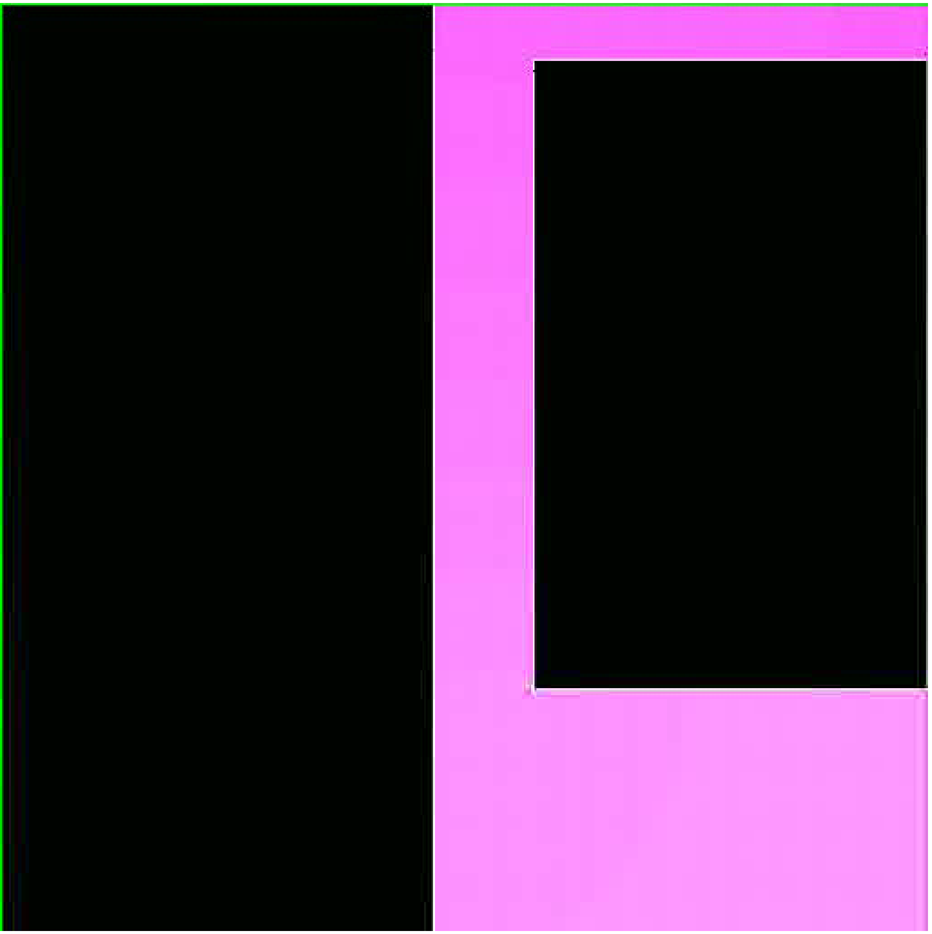
- Electrokinetically driven flow
- Joule heating
- Heat Transfer influences performance
- Elmer as a tool for prototyping
- Complex geometry
- Complex simulation setup



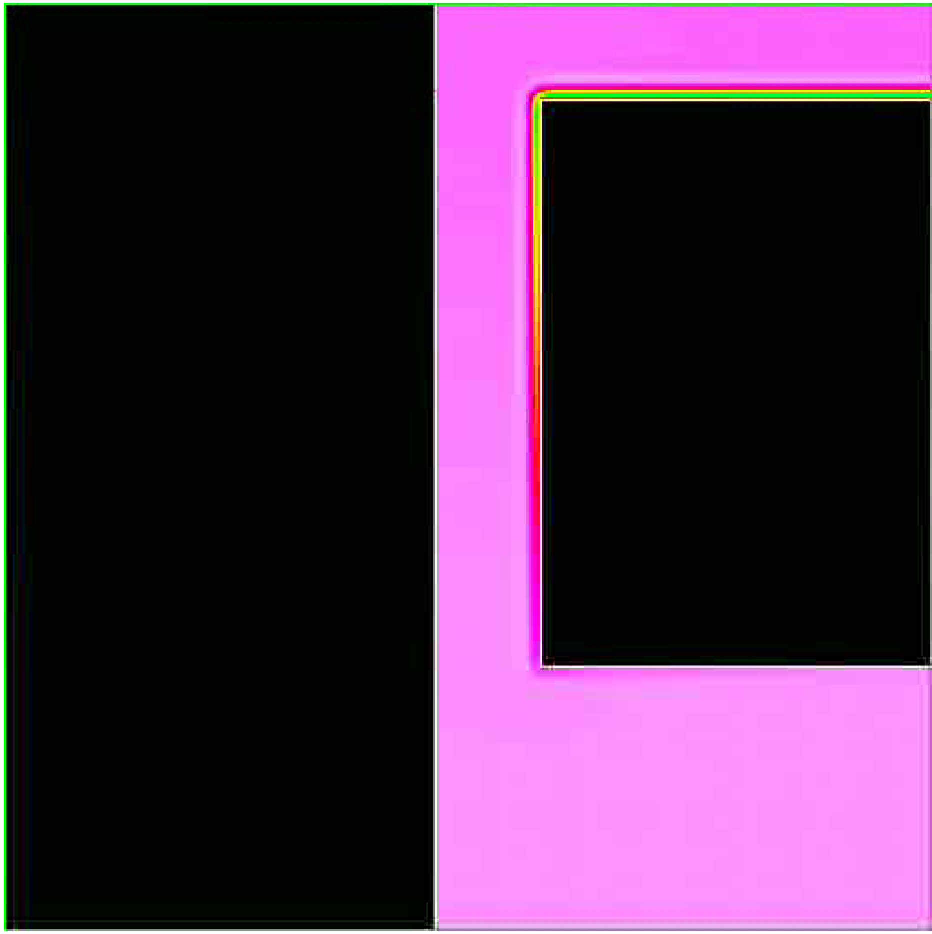
T. Sikanen, T. Zwinger, S. Tuomikoski, S. Franssila, R. Lehtiniemi, C.-M. Fager, T. Kotiaho and A. Pursula, Microfluidics and Nanofluidics (2008)

Acoustics: Losses in small cavities

Temperature waves resulting from the Helmholtz equation



Temperature waves computed from the linearized Navier-Stokes equation

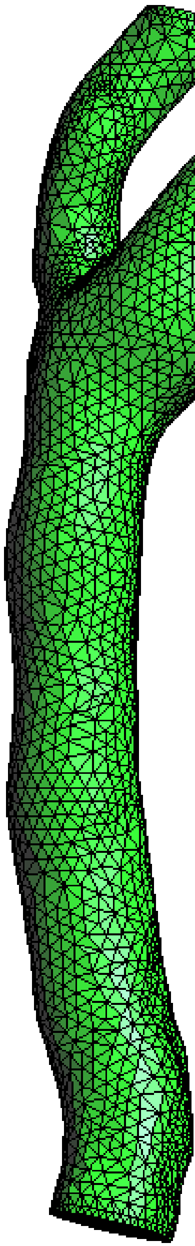


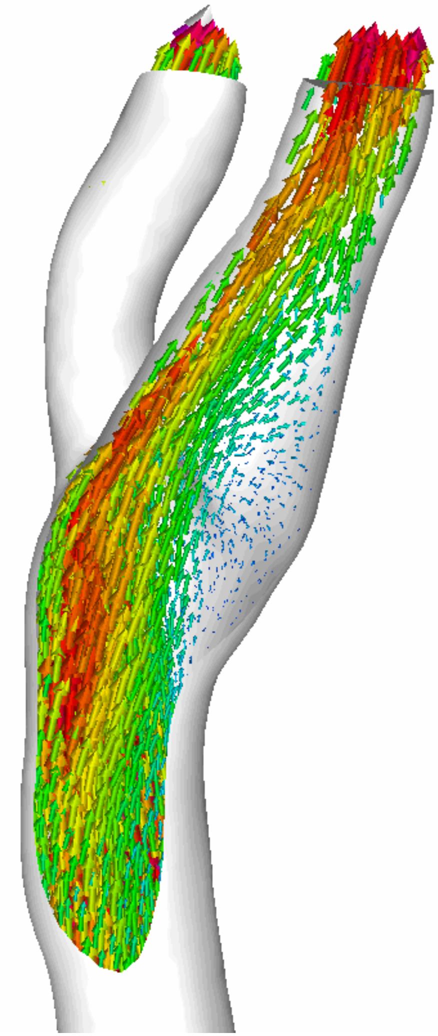
M. Malinen, *Boundary conditions in the Schur complement preconditioning of dissipative acoustic equations*, SIAM J. Sci. Comput. 29 (2007)

Computational Hemodynamic

- 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

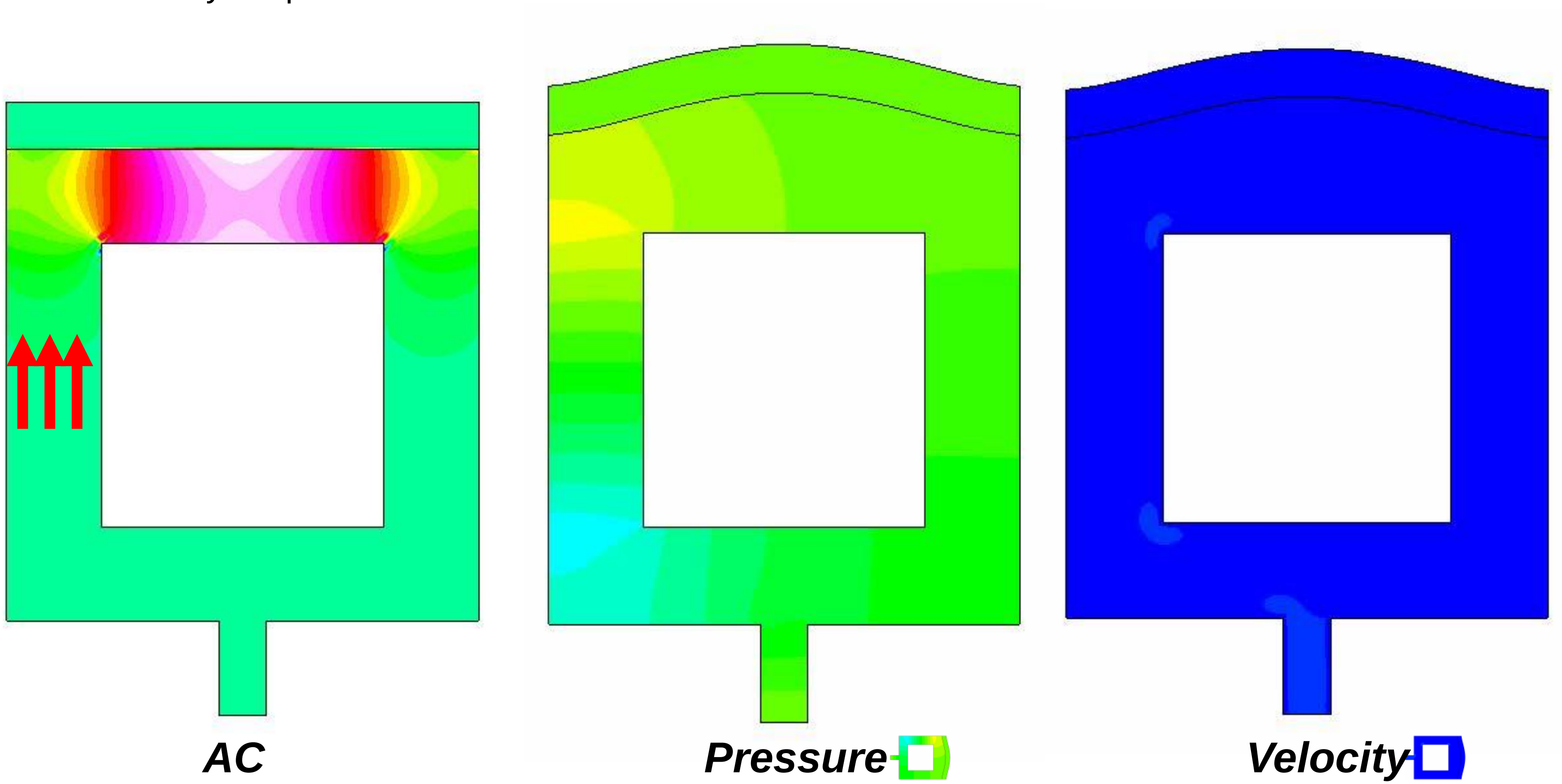




Blood flow in carotid artery accounting FSI interaction

FSI with articifical compressibility

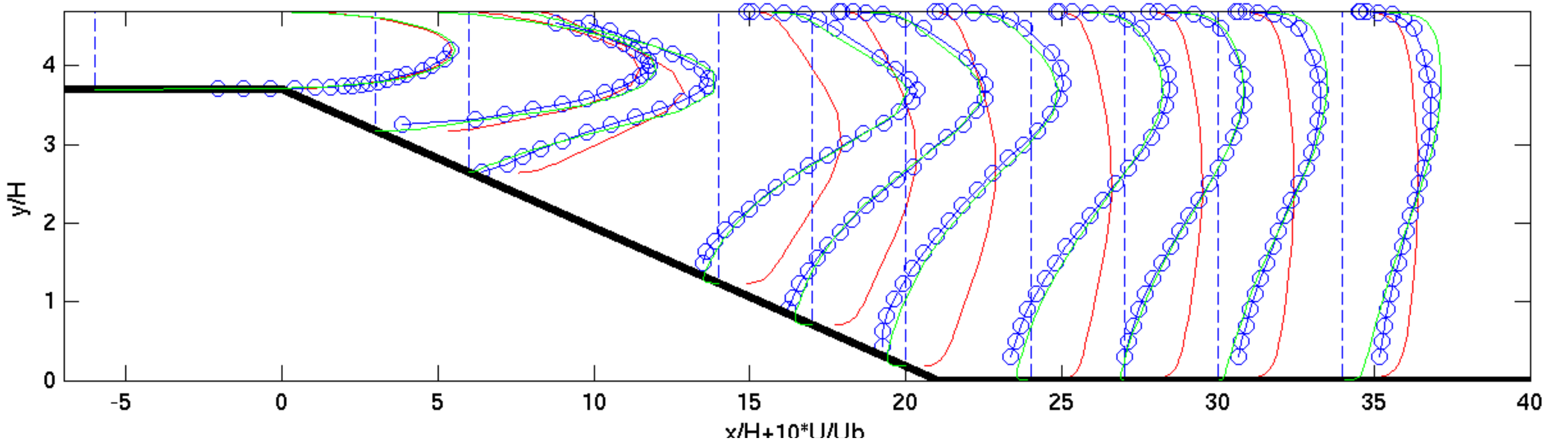
- Flow is initiated by a constant body force at the left channel
- Natural boundary condition is used to allow change in mass balance
- An optinmal artificial compressibility field is used to speed up the convergence of loosely coupled FSI iteration



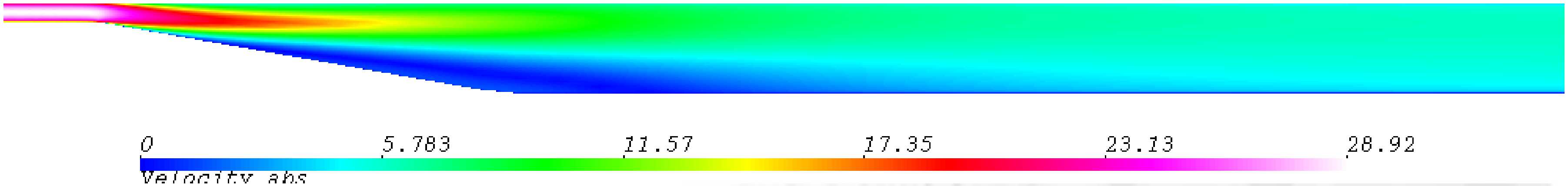
P. Råback, E. Järvinen, J. Ruokolainen, *Computing the Artificial Compressibility Field for Partitioned Fluid-Structure Interaction Simulations,* ECCOMAS 2008

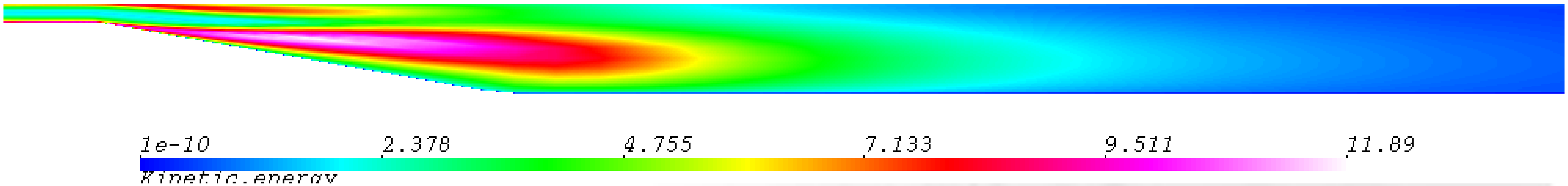
RANS turbulence modeling

Comparison of *k*-ε vs. v^2-*f* –turbulence models (red



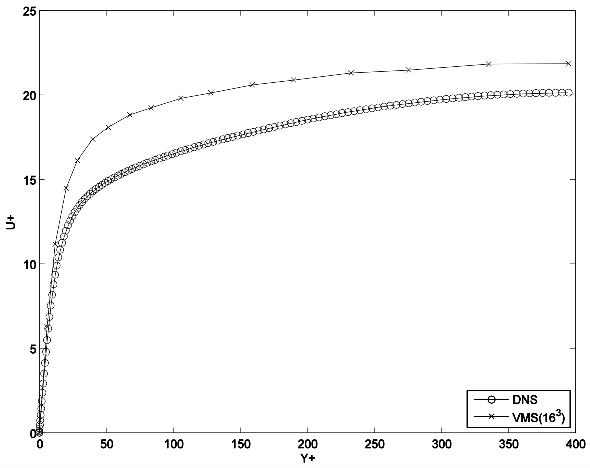
Simulation J. Ruokolainen, CSC



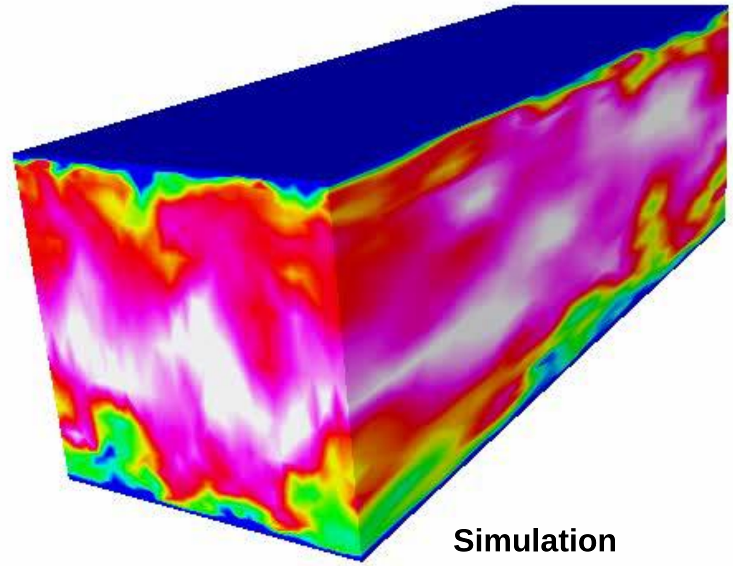


VMS turbulence modeling

- 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



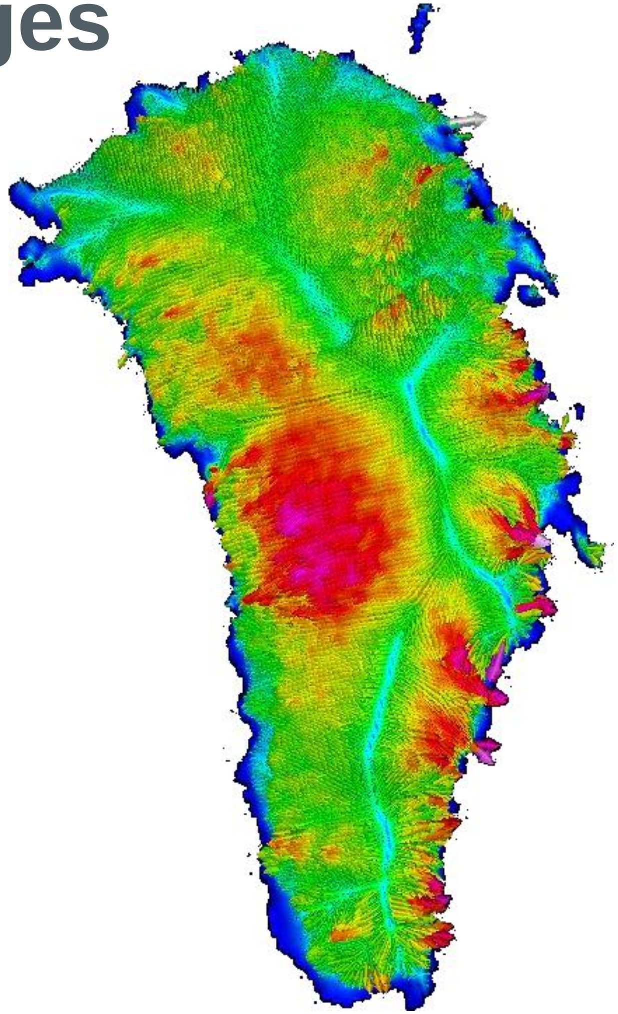
Plane flow with Re_τ=395

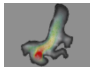


Simulation
J. Ruokolainen, CSC

Glaciology: Grand challenges

- Elmer is the leading code for 3D ice flow simulation even internationally
- Elmer uses full Stokes equation to model the flow
- Currently the mostly used tool in the area
  - British Antarctic Survey
  - University of Grenoble
  - University of Sapporo
- Simulations of continental ice sheets very demanding
- Climate change makes the simulations very important





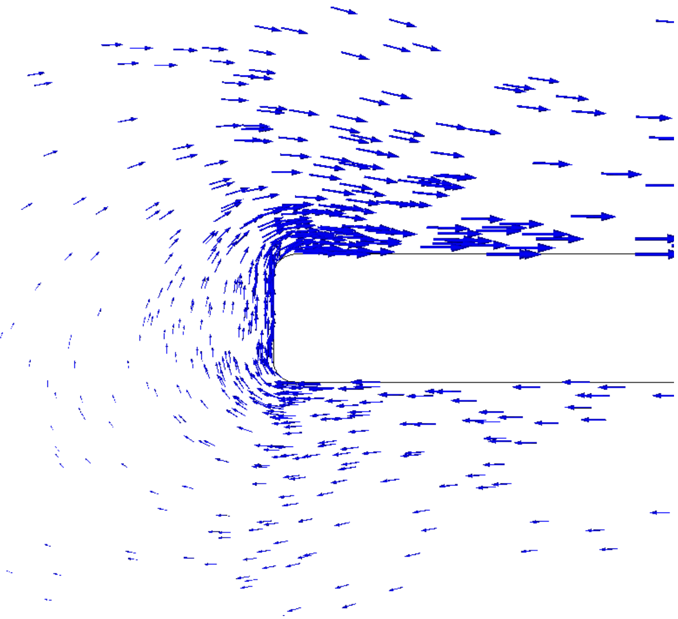
Simulation T. Zwinger, CSC

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



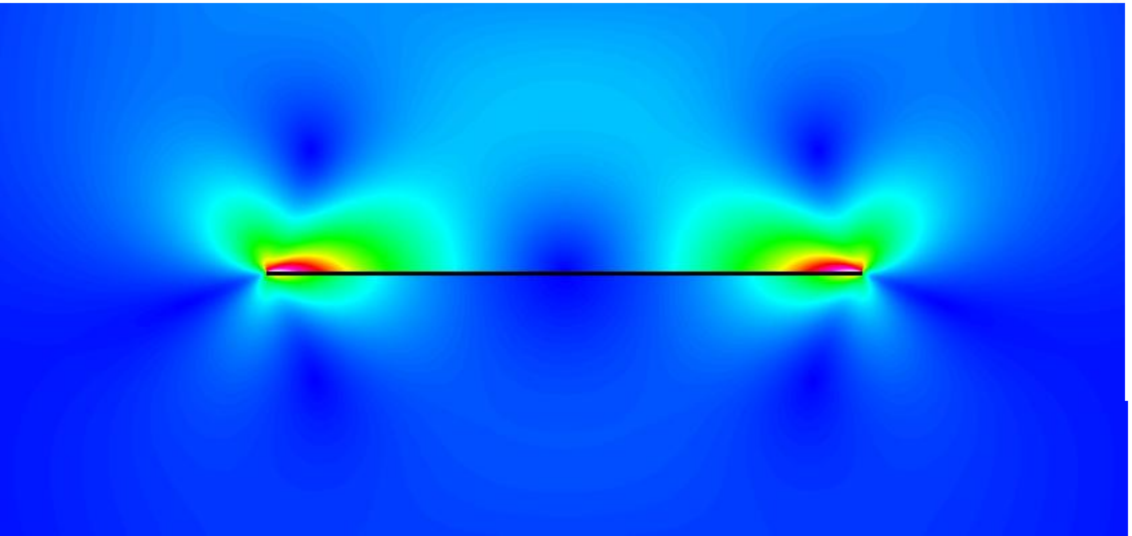
2D compressible Navier-Stokes eq. with heat eq. plus two rarefied gas effects:

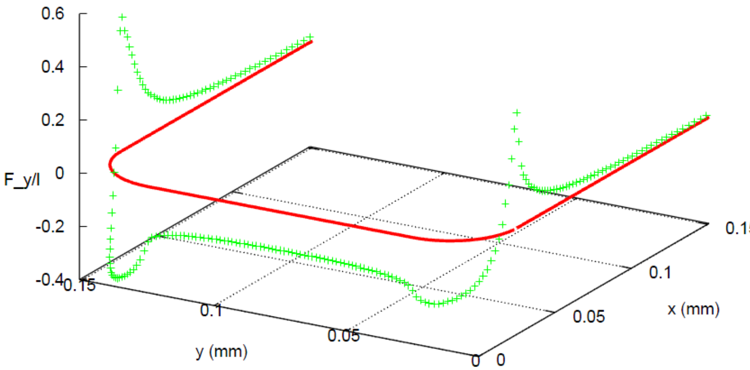
- Maxwell's wall slip and thermal transpiration

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

- Smoluchowski's temperature jump

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

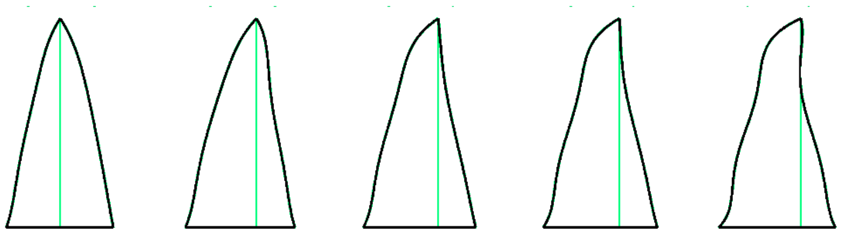




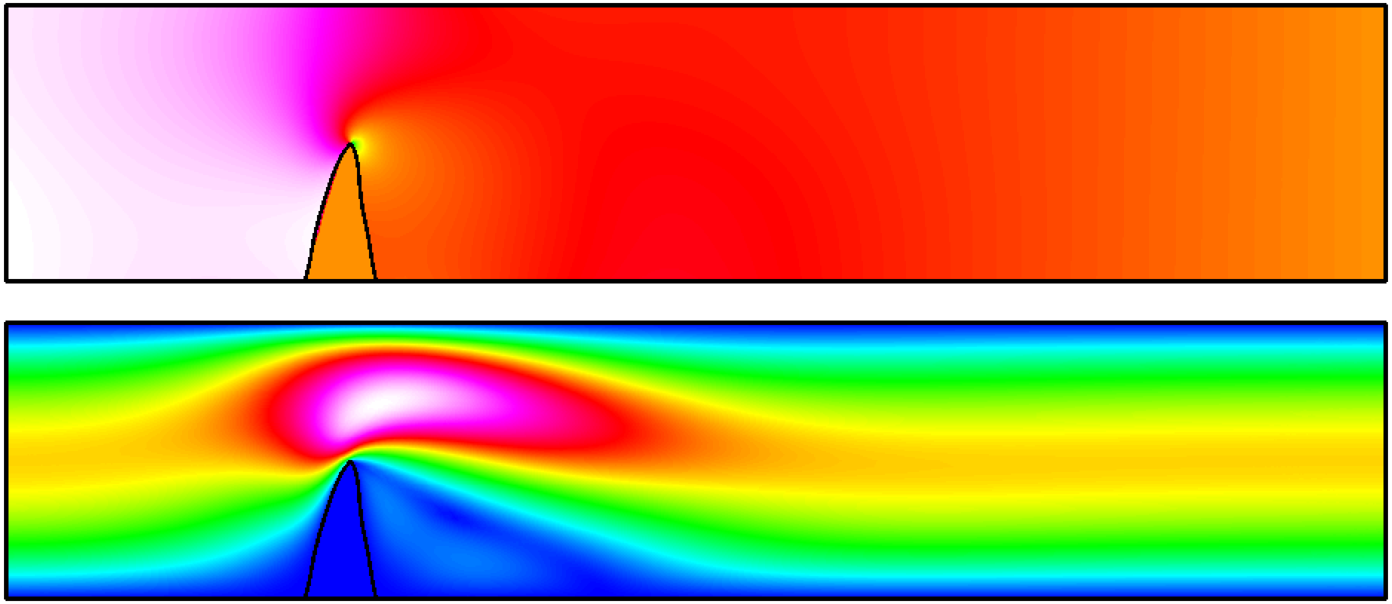
Simulation Moritz Nadler, 2008

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



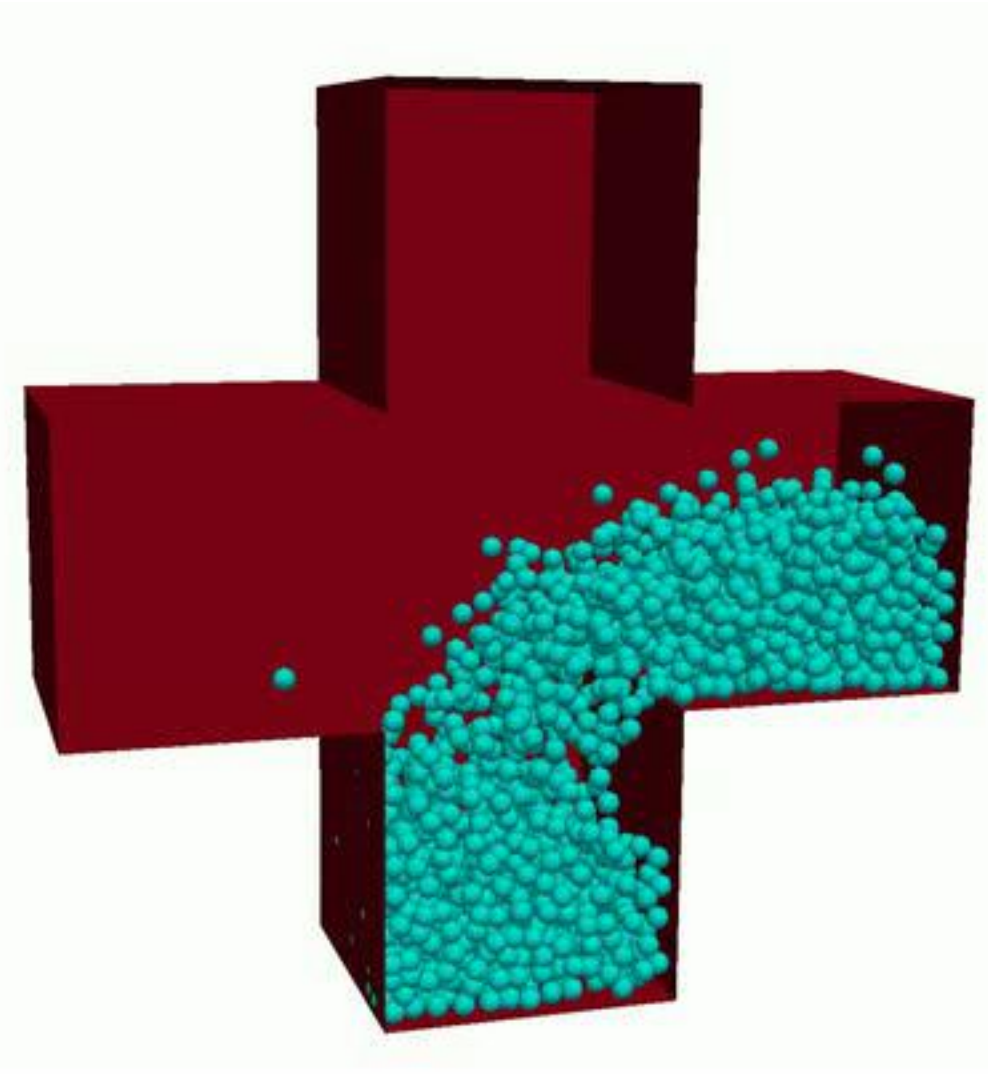
Optimized profiles for Re={0,10,50,100,200}



Pressure and velocity distribution with Re=10

Simulation Peter Råback

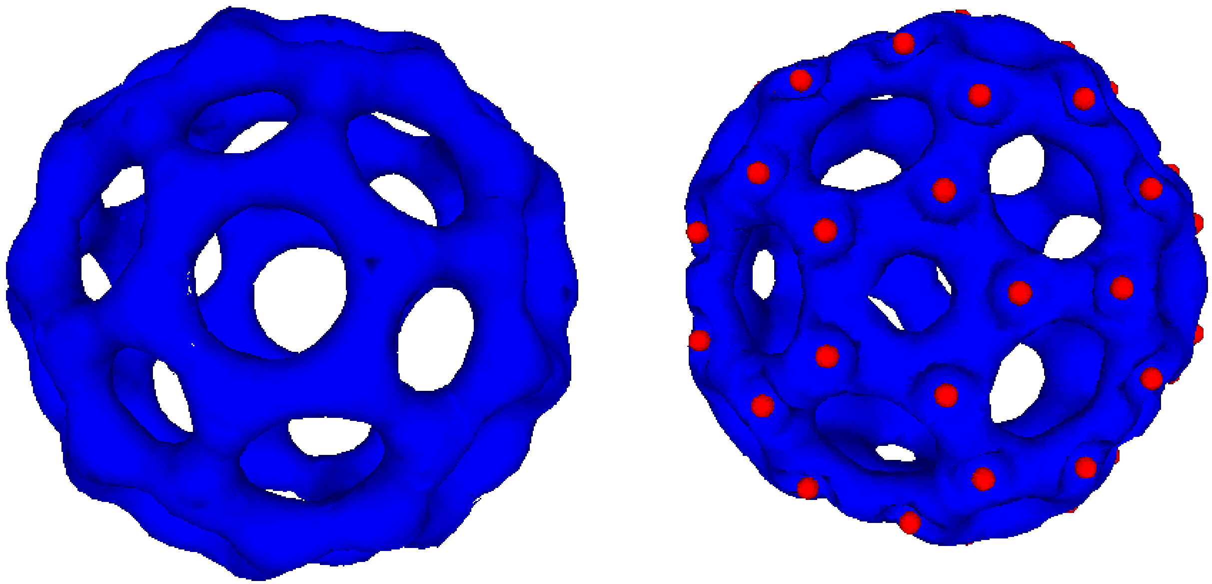
Particle tracker - Granular flow



Quantum Mechanics

- Finite element method is used to solve the Kohn-Sham equations of density functional theory (DFT)

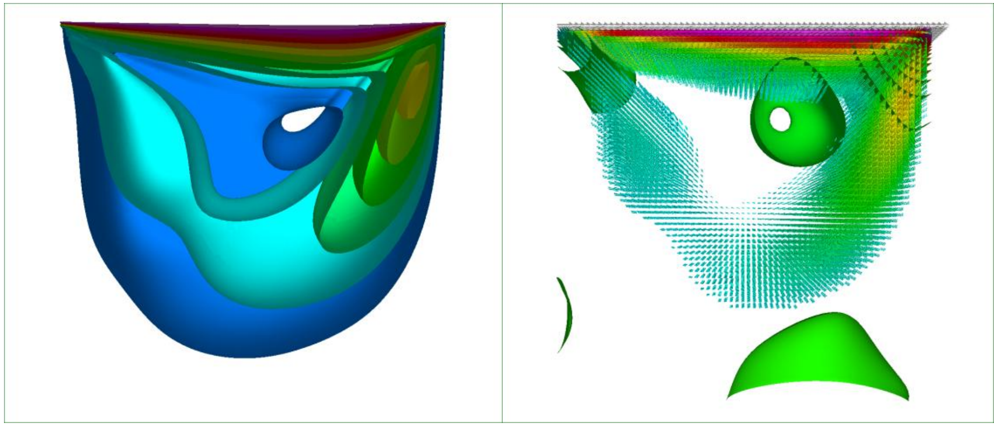
- Charge density and wave function of the 61st eigenmode of fullerine C60
- All electron computations using 300 000 quadratic tets and 400 000 dofs



Simulation Mikko Lyly, CSC

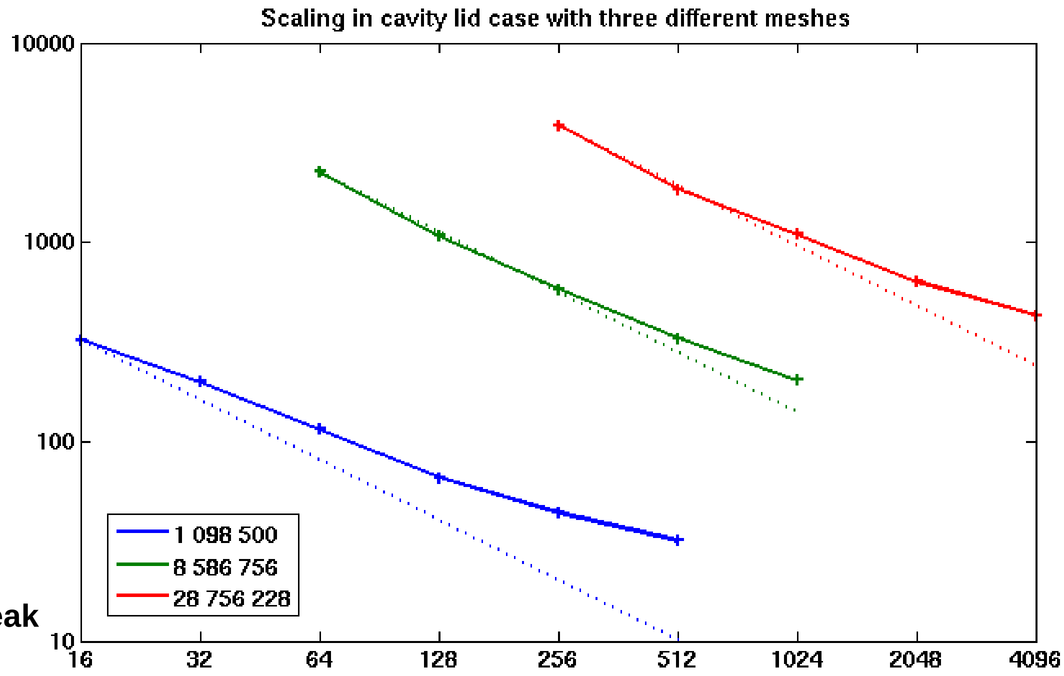
Parallel performance

- Partitioning by Metis or simple geometric division
- Parallel assembly and solution by GMG or Krylov subspace methods.
- Parallel performance may scale up to thousands of cores
- Simulation with over one billion unknowns has been performed



Scaling of wall clock time with dofs in the cavity lid case using GMRES+ILU0. Simulation Juha Ruokolainen, CSC, visualization Matti Gröhn, CSC .

Louhi: Cray XT4/XT5 with 2.3 GHz 4-core AMD Opteron. All-in-all 9424 cores and Peak power of 86.7 Tflops.



FETI Parallel performance

Procs	Time (s)	Iters
27	10.52	26
64	12.30	29
125	9.27	31
216	9.96	31
343	10.26	32
512	11.18	32
729	12.13	33
1000	19.88	33
3375	31.52	35

Naviers equation in a unit cube with constant loading from the side.

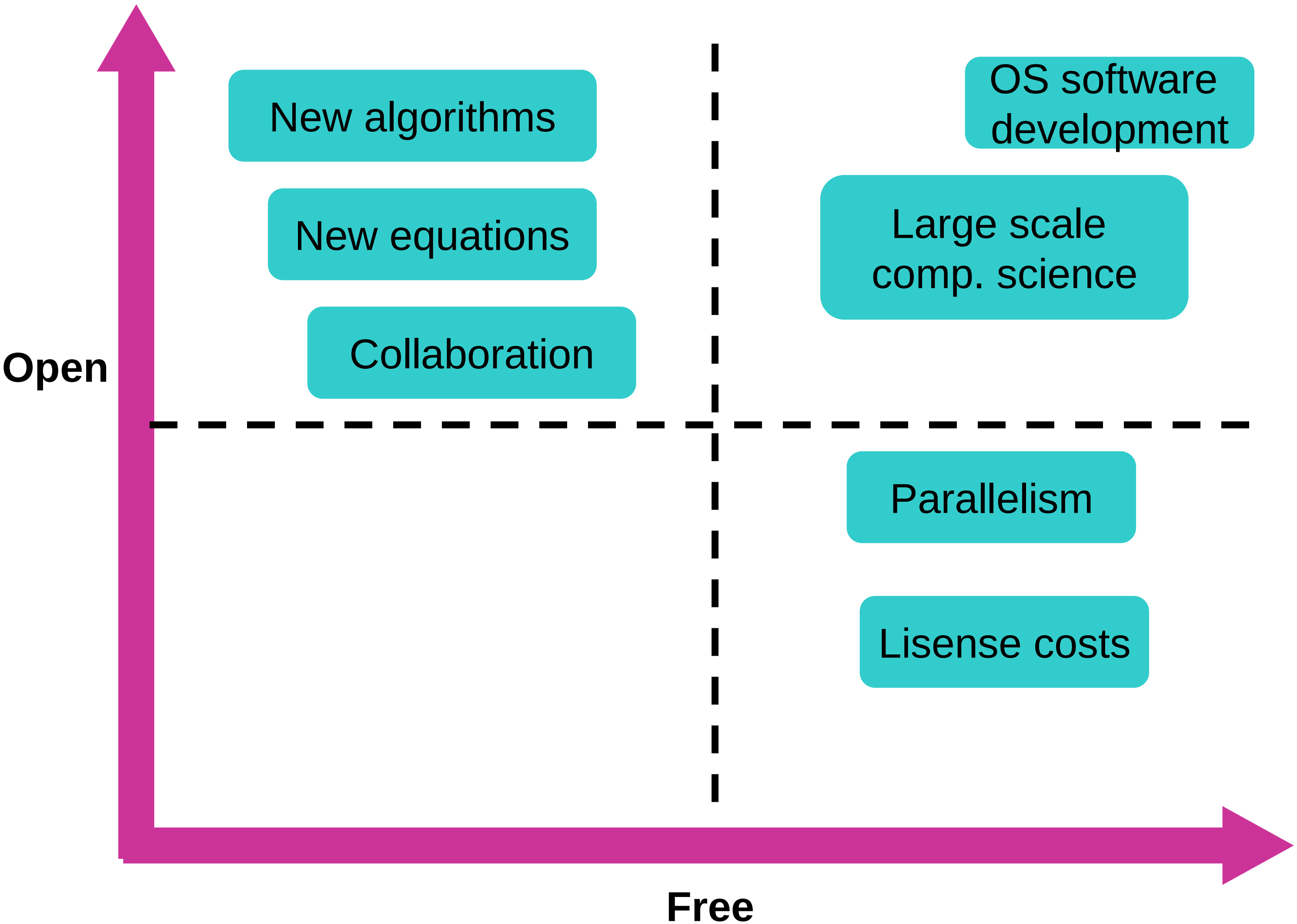
The size of the case was kept fixed at 8000 elements for each partition.

The largest case includes thus around 80 Mdofs.

Computations carried out on Curie (CAE) in 2011

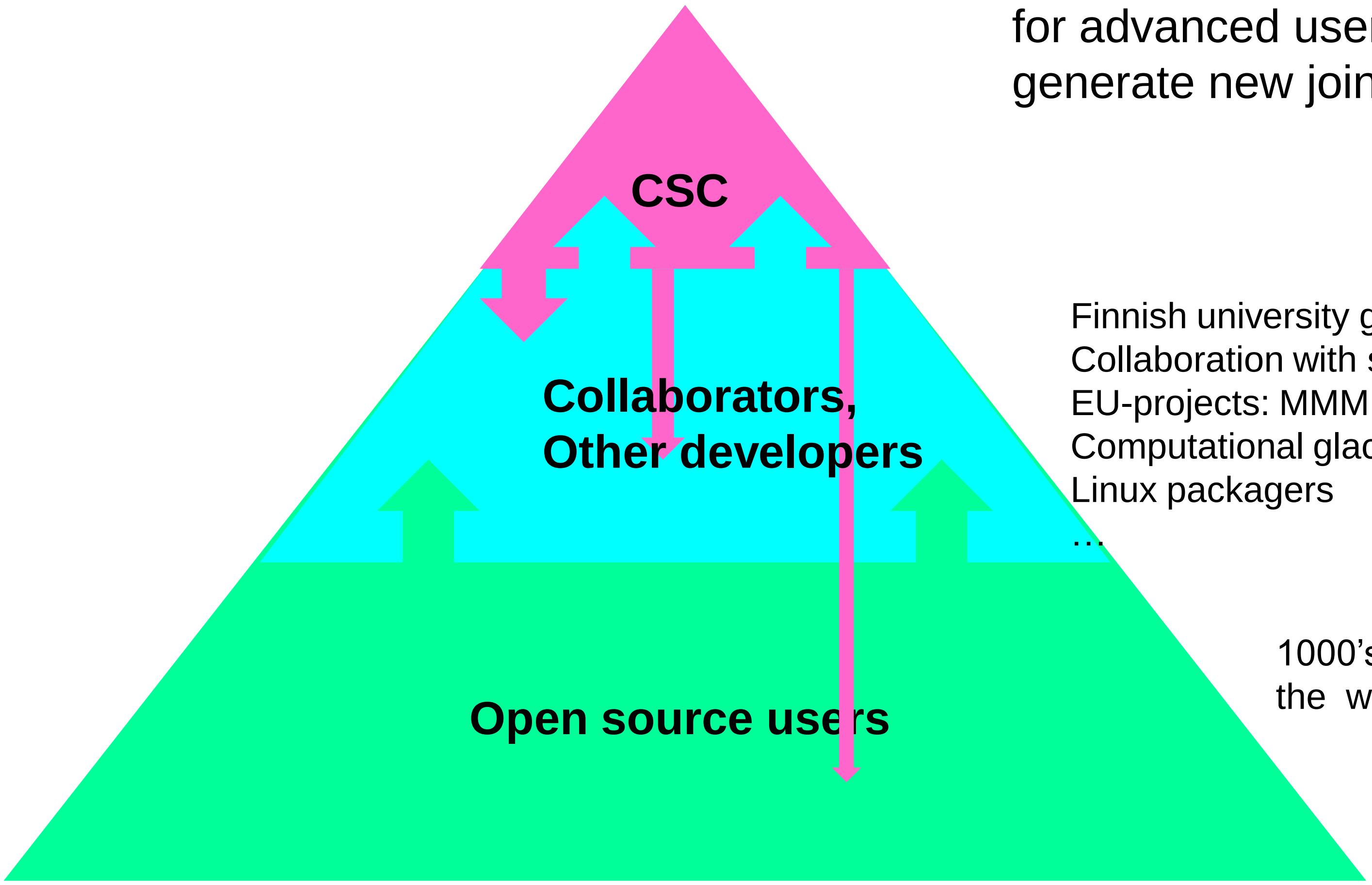
Reasons to use open source software

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



Ecosystem of Elmer

GOAL: make Elmer more attractive for advanced users and thereby generate new joint projects



Finnish university groups
Collaboration with selected companies
EU-projects: MMM@HPC, PRACE,…
Computational glaciology,
Linux packagers
…

1000’s of users around
the world (basic & advanced)

Most important Elmer resources

- http://www.csc.fi/elmer
  - Official Homepage of Elmer
  - Overview, examples, compilation, …
  - pointers to other sources of information
- http://sourceforge.net/projects/elmerfem/
  - Version control system: svn
  - Binaries
- www.elmerfem.org
  - Discussion forum & wiki
- Further information: Peter.Raback@csc.fi

- Thank you for your attention!