

Elmer – an Open Source Finite Element Software for Multiphysical Problems

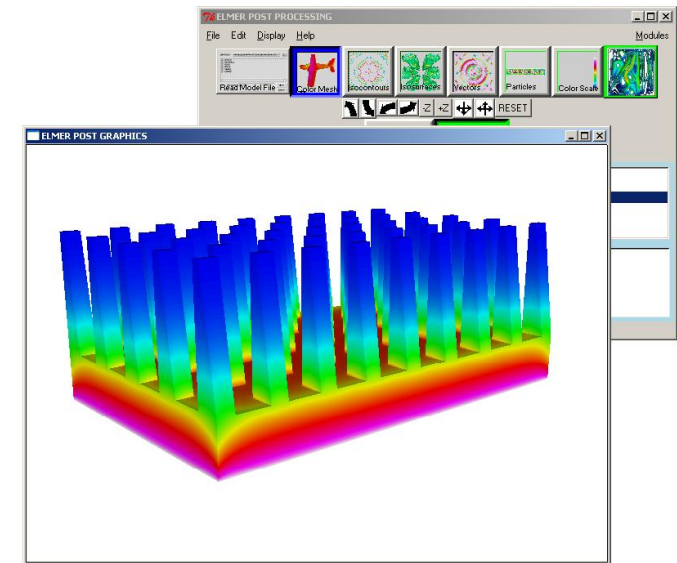
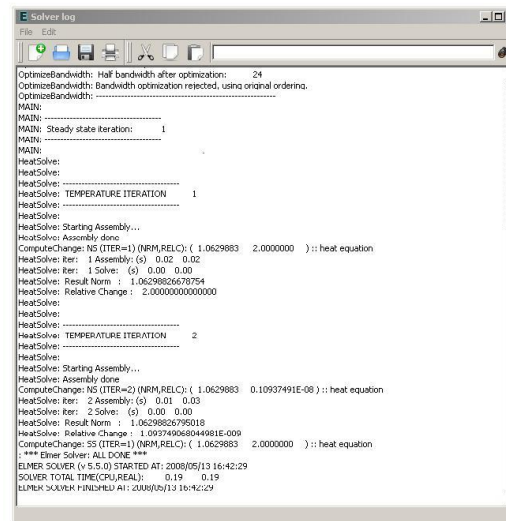
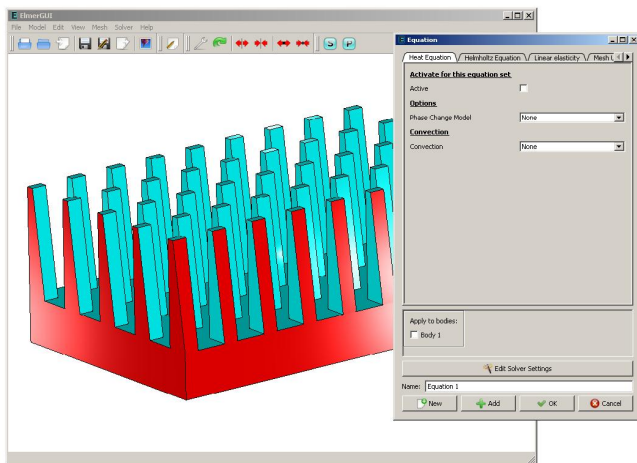
Peter Råback

CSC, Finnish IT Center for Science

Elmer Basic Course, 28th May 2008, CSC, Espoo



Elmer – A finite element software for multiphysical problems

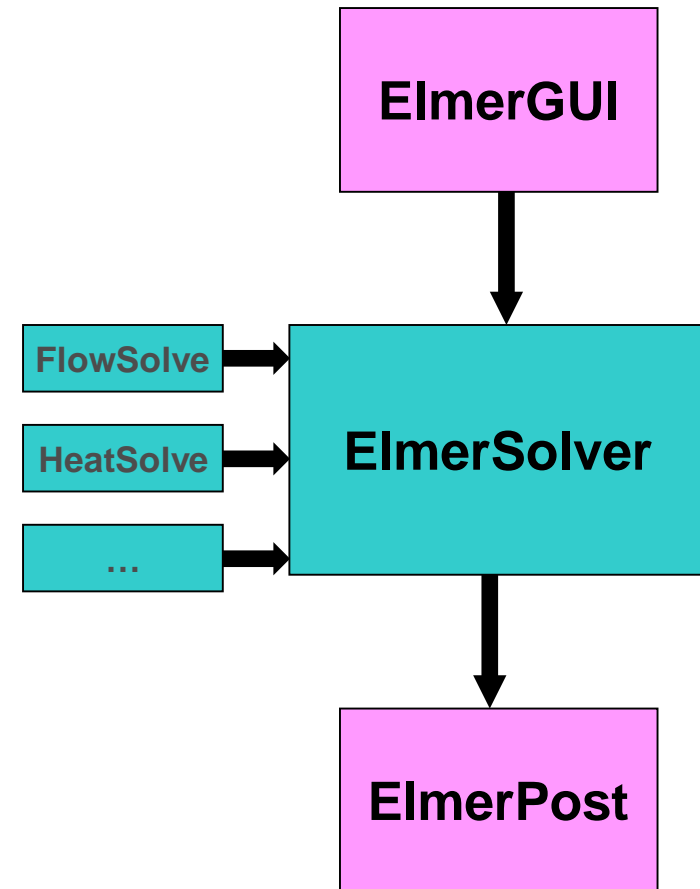


ElmerGUI + ElmerSolver + ElmerPost
ElmerGrid
ElmerFront



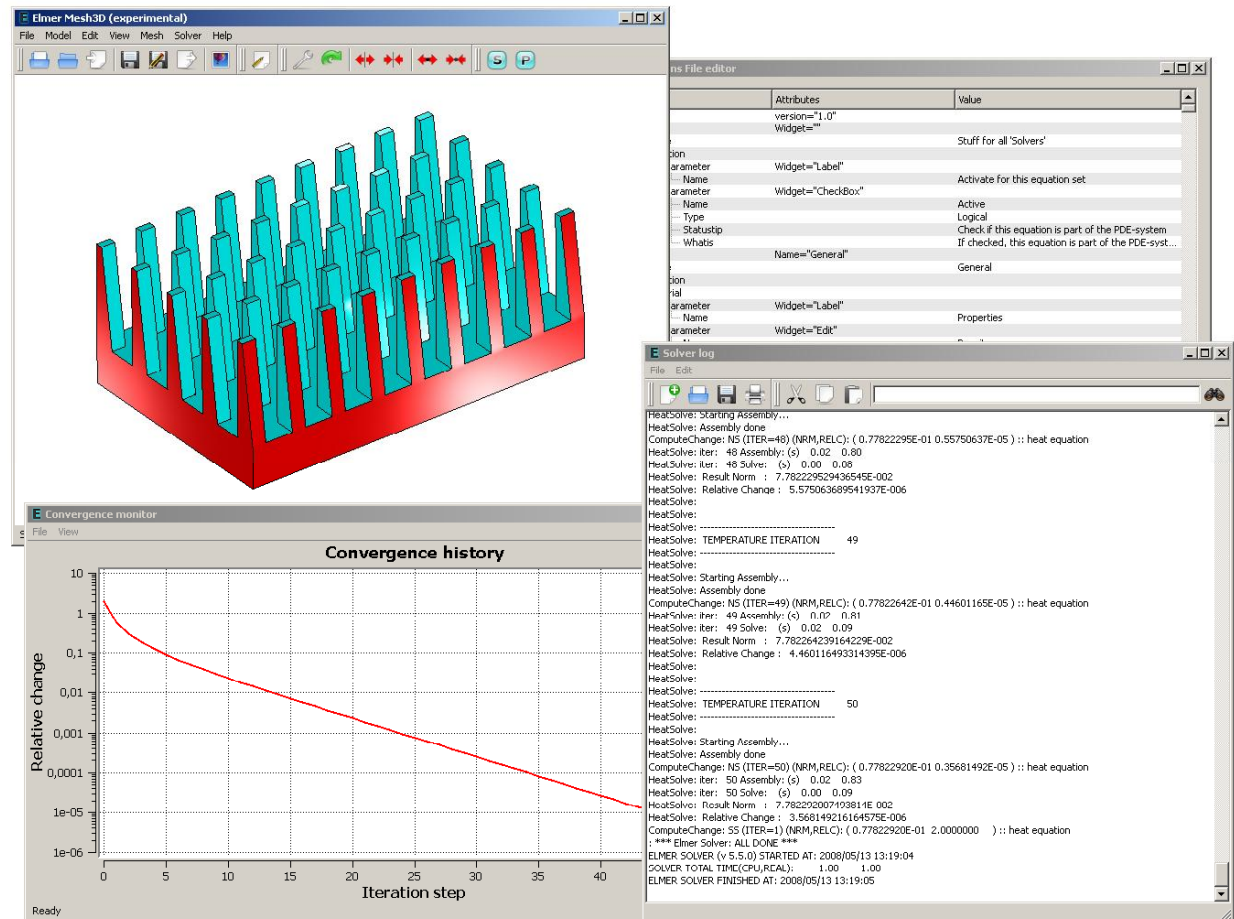
Components of Elmer software suite

- **Elmer is actually a suite of several programs**
- **You may use many of the components independently**
- **Preprocessing**
 - ElmerGUI (uses ElmerGrid, netgen, tetgen)
- **ElmerSolver**
- **Post-processing**
 - ElmerPost
- **Others**
 - ElmerFront: the old preprocessor
 - Mesh2D: Delaunay mesher usable through ElmerFront
 - MATC: library for on-the-fly arithmetics
 - ElmerGrid as a stand-alone tool
 - 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 2008
- **Mesh generation**
 - 3D Delaunay mesh generation by tetgen and netgen
 - Simple mesh generation and mesh import by ElmerGrid
- **Easiest tool for case specification**
 - Even educational use
- **New solvers easily supported through GUI**
 - XML based menu definition



ElmerSolver

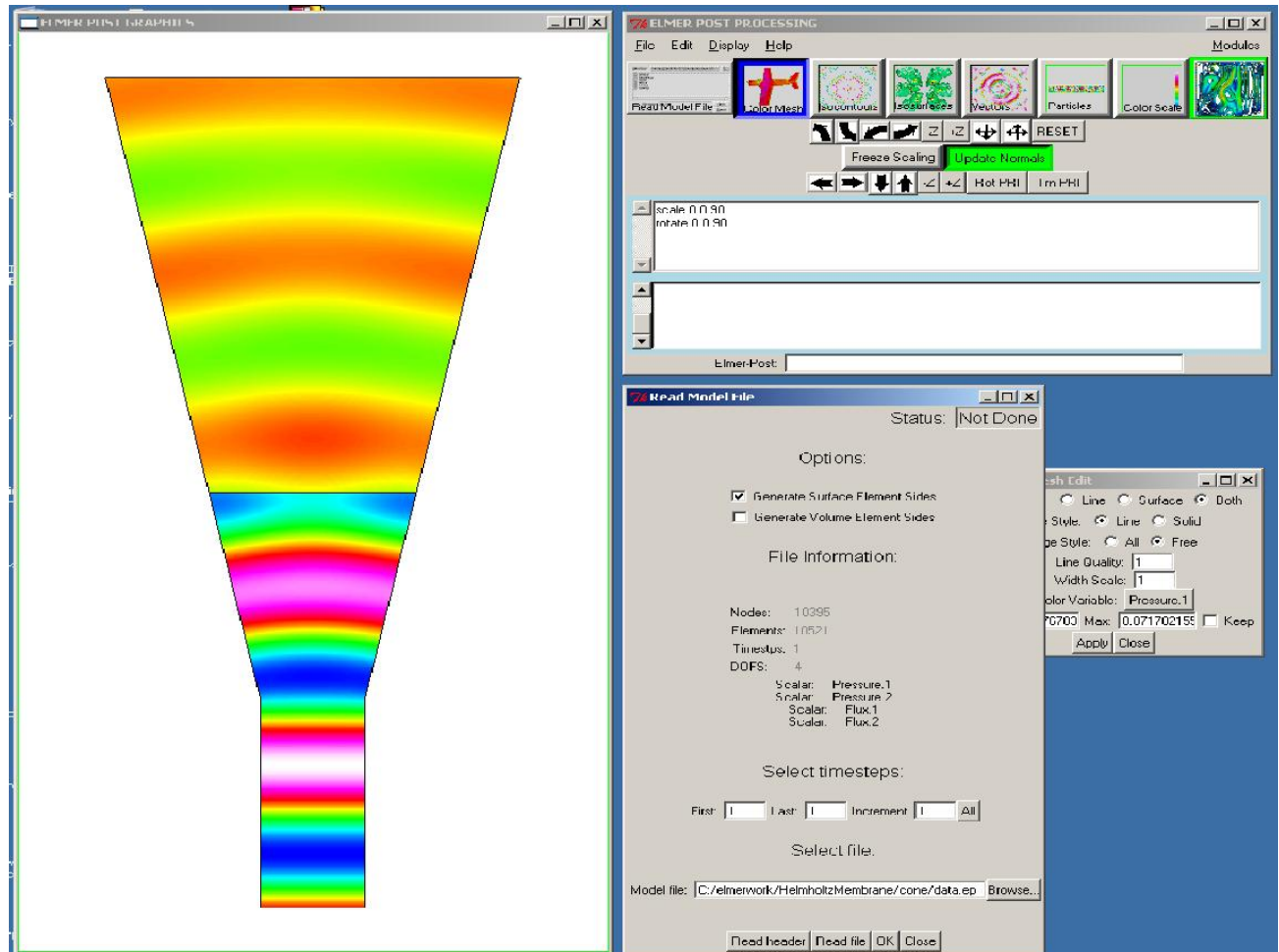
- **Assembly and solution of the finite element equation**
- **Partitioned operation with iterative solvers**
- **Note: When we talk of Elmer we mainly mean ElmerSolver**

```
> ElmerSolver StepFlow.sif
MAIN: =====
MAIN:  E L M E R  S O L V E R  S T A R T I N G
MAIN:  Library version: 5.3.2
MAIN: =====
MAIN:
MAIN: -----
MAIN: Reading Model ...
...
...
SolveEquations: (NRM,RELC): ( 0.34864185 0.88621713E-06 ) :: navier-stokes
: *** Elmer Solver: ALL DONE ***
SOLVER TOTAL TIME(CPU,REAL):          1.54          1.58
ELMER SOLVER FINISHED AT: 2007/10/31 13:36:30
```



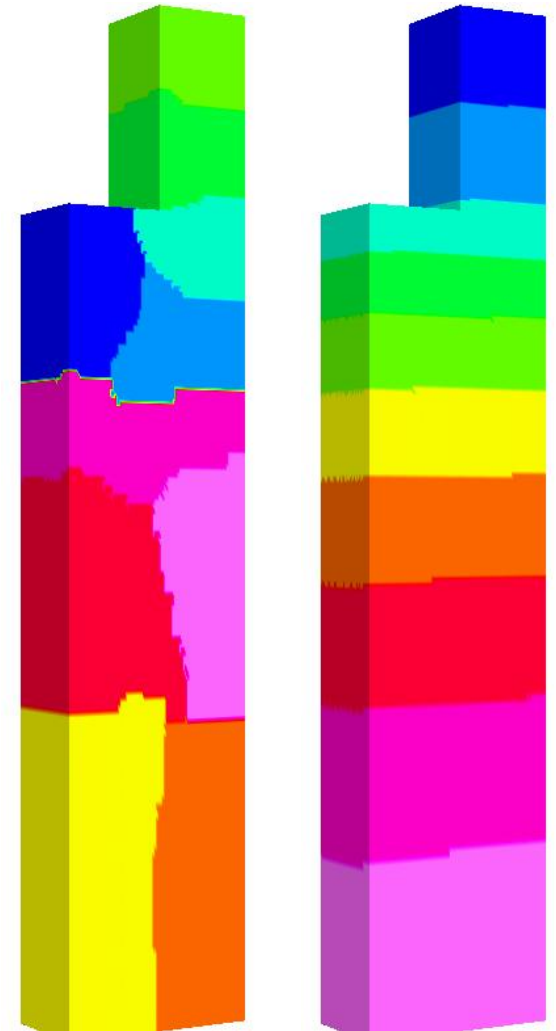
ElmerPost

- **Based on the FUNCS program**
 - written in late 80's and early 90's by Juha Ruokolainen
- **All basic presentation types**
 - Colored surfaces and meshes
 - Contours, isosurfaces, vectors, particles
 - Animations
- **Includes MATC language**
 - Data manipulation
 - Derived quantities
- **Output formats**
 - ps, ppm, jpg, mpg
 - animations



ElmerGrid

- **Creation of 2D and 3D structured meshes**
 - Rectangular basic topology
 - Extrusion, rotation
 - Simple mapping algorithms
- **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, discontin. BC,...)



Alternative mesh generators for Elmer

Open Source tools

- **Mesh2D**
 - 2D Delaunay
 - Writes Elmer format
 - Usable via the old ElmerFront
- **ElmerGrid: native to Elmer**
 - Simple structured mesh generation
 - Usable via ElmerGUI
- **Tetgen, Netgen**
 - Tetrahedral mesh generation
 - Usable via ElmerGUI as a plug-in
- **Gmsh**
 - Includes geometry definition tools
 - ElmerGUI/ElmerGrid can read the format
- **Triangle**
 - 2D Delaunay
 - ElmerGUI/ElmerGrid can read the format
- ...

Commercial tools

- **GiD**
 - Inexpensive
 - With an add-on module can directly write Elmer format
- **Gambit**
 - Preprocessor of Fluent suite
 - ElmerGUI/ElmerGrid can read .FDNEUT format
- **Comsol multiphysics**
 - ElmerGUI/ElmerGrid can read .mpltxt format
- ...

- **Ask for your format:
Writing a parser from ascii-mesh
file usually not big a deal**

Alternative postprocessors for Elmer

Open Source tools

- **ElmerPost**
 - Postprocessor of Elmer suite
- **ParaView, Visit**
 - Use ResultOutputSolve to write .vtu or .vtk
 - Visualization of parallel data
- **OpenDX**
 - Supports some basic elementtypes
- **Gmsh**
 - Use ResultOutputSolve to write dat
- **Gnuplot, R, Octave**
 - Use SaveData to save results in ascii matrix format
 - Line plotting

Commercial tools

- **Matlab, Excel**
 - Use SaveData to save results in ascii matrix format
 - Line plotting

Elmer - Physical Models

- **Heat transfer**
 - Heat equation
 - Radiation with view factors
 - convection and phase change
- **Fluid mechanics**
 - Navies-Stokes (2D & 3D)
 - Turbulence models: $k-\varepsilon$, v^2-f
 - Reynolds (2D)
- **Structural mechanics**
 - Elasticity (anisotropic, 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**
 - Electrostatics
 - Magnetic vector potential
- **Electrokinetics**
 - Poisson-Boltzmann
 - Poisson-Nernst-Planck
- **Quantum mechanics**
 - DFT (Kohn Scham)
-

Elmer – numerical methods

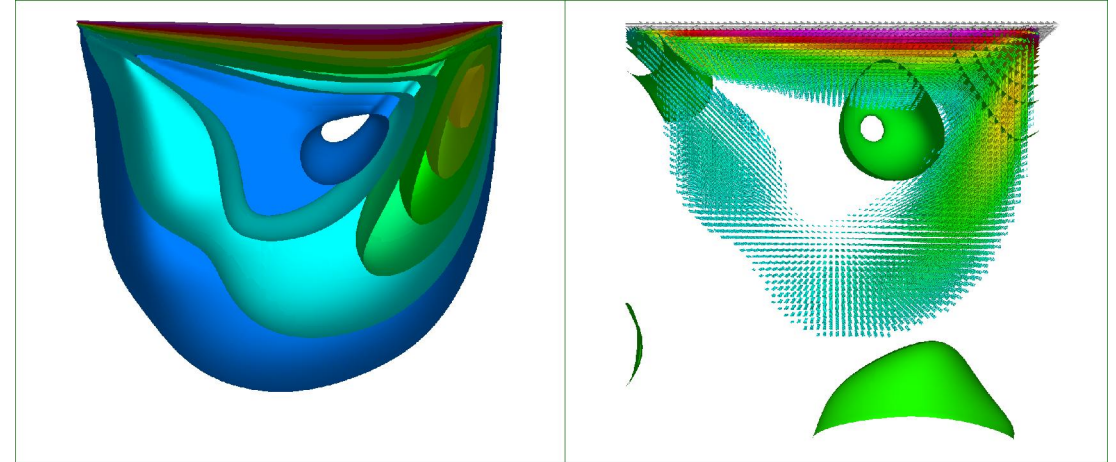
- **Time-dependency**
 - Static, transient, eigenmode analysis
- **Discretization**
 - Galerkin, Discontinuous Galerkin (DG)
 - Stabilization: SUPG, bubbles
 - Lagrange, edge, face, and p-elements
- **Matrix equation solvers**
 - Direct: Lapack, Umfpack
 - Iterative Krylov space methods
 - multigrid solvers (GMG & AMG) for “easy” equations
- **Parallelism**
 - Parallel assembly and solution with iterative methods
- **Adaptivity**
 - For selected equations, works well in 2D

Parallel performance

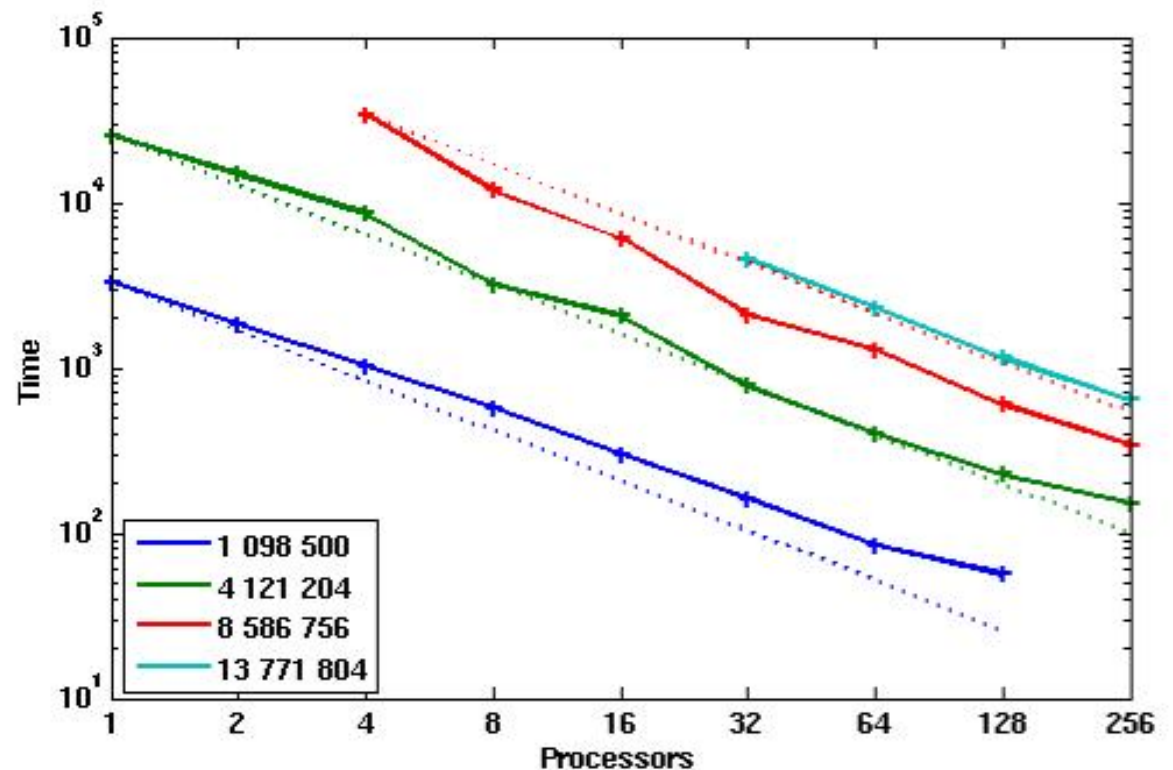
- Partitioning by Metis or simple geometric division
- Parallel assembly and solution by GMG or Krylov subspace methods.
- Parallel performance scales often well up to hundreds of processors
- Simulation with over one billion unknowns has been performed



HP ProLiant with 2048 compute cores (AMD Opteron Dual Core 2.6 GHz).



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

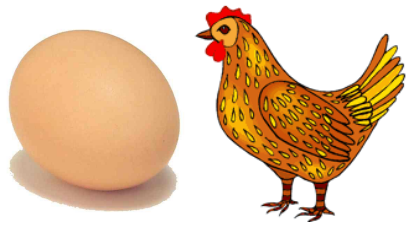


Some possible multiphysical combinations

Equation	Field	T	v	E, B	c	u
Energy	Temperature, T	-				
Navier-Stokes	Velocity, v	1	-			
Maxwell's	Electric & magnetic, E, B	2	3	-		
Diffusion, Reaction	Concentration, c	4	5	6	-	
Elasticity	Displacement, u	7	8	9	10	-

1. Thermal flow: natural convection
2. Thermal-electrical: Heating by induction
3. Magnetohydrodynamics, Electrokinetics
4. Temperature dependent chemical reactions and diffusion
5. Reactive flow: CFD, combustion
6. Electrochemistry: batteries, electrodes, surface treatment
7. Thermoelasticity and –plasticity
8. Fluid-structure interaction: hemodynamics
9. Electro-mechanical: MEMS, piezoelectricity
10. Growth phenomena

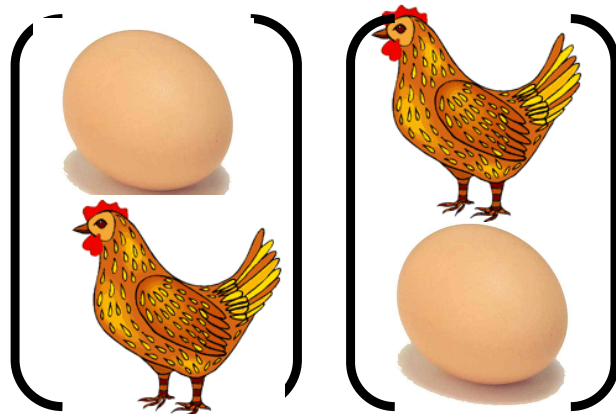
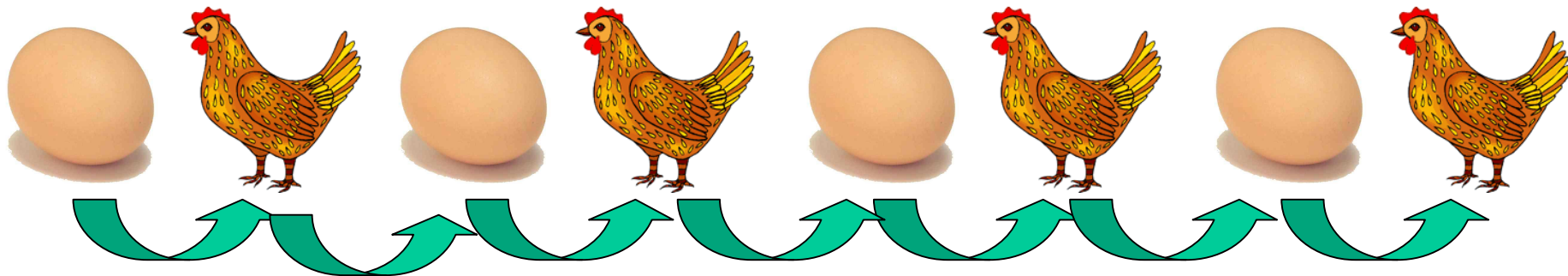
Solution strategies for coupled problems



Hierarchical solution



Iterative solution



Monolithic solution

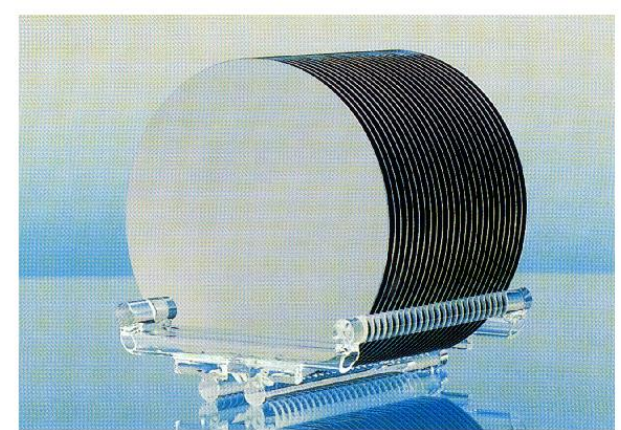


Most important Elmer resources

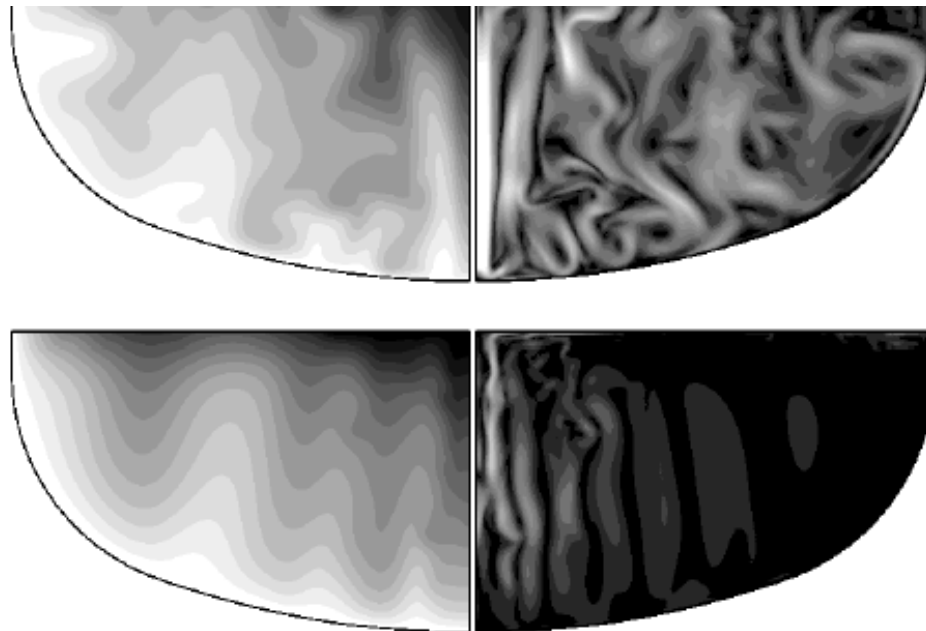
- <http://www.csc.fi/elmer>
 - Official Homepage of Elmer
 - Overview, examples, compilation, ...
 - pointers to other sources of information
- <http://sourceforge.net/projects/elmerfem/>
 - Version control system: svn
 - Binaries, wiki, ...
- elmerdiscussion@postit.csc.fi
 - Discussion forum

Czochralski Crystal Growth

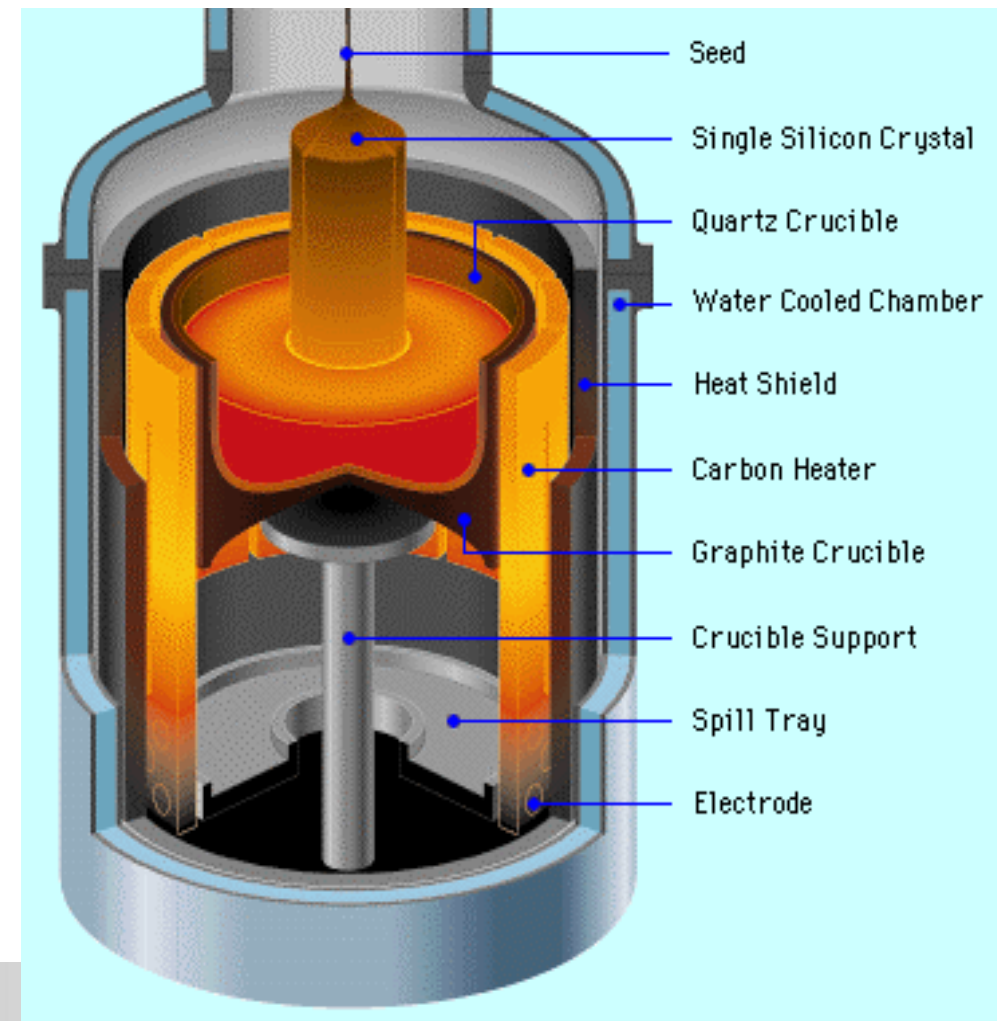
- Most crystalline silicon is grown by the Czochralski (CZ) method
- One of the key application when Elmer development was started in 1995



Figures by Okmetic Ltd.



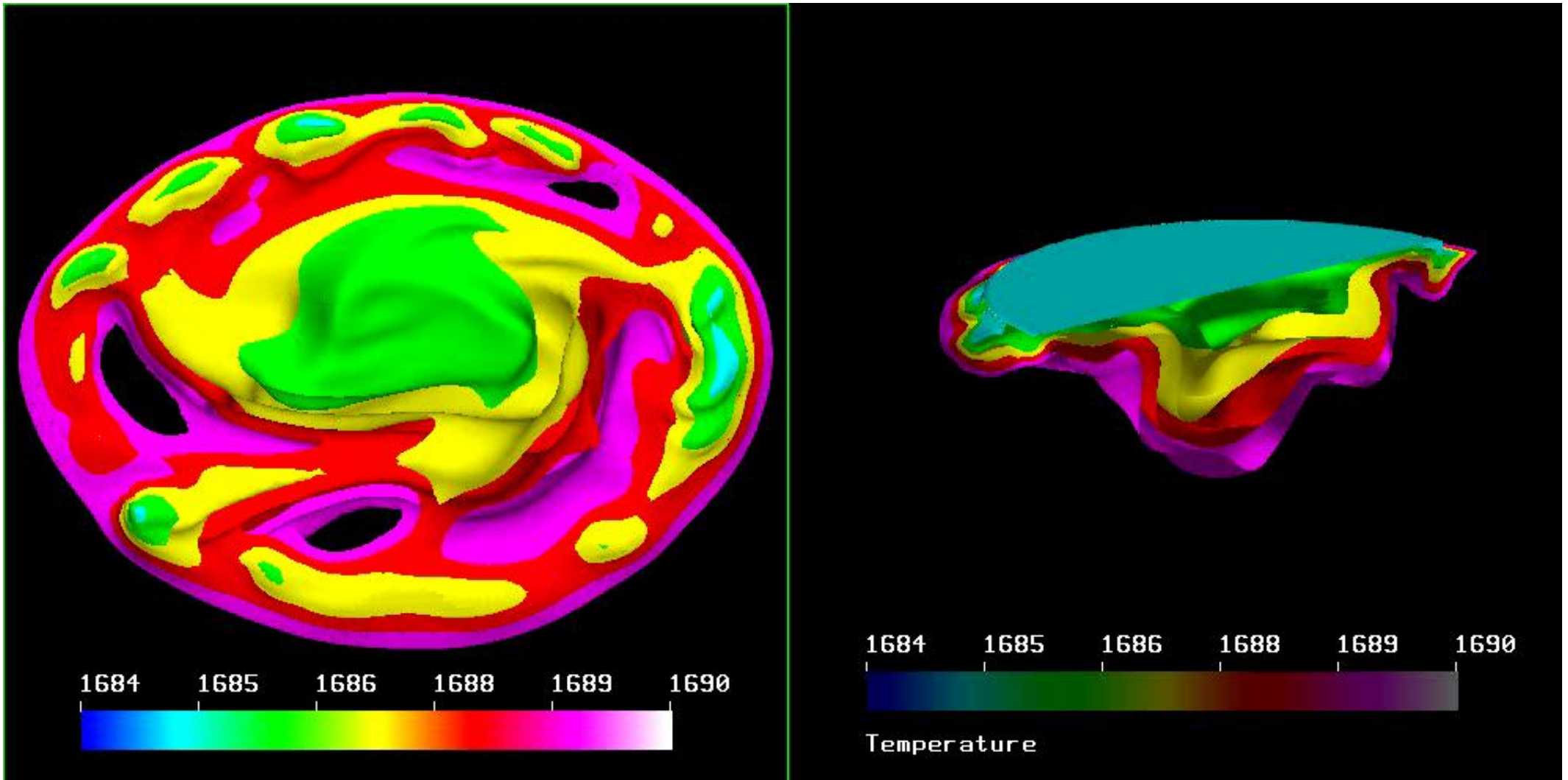
V. Savolainen et al., *Simulation of large-scale silicon melt flow in magnetic Czochralski growth*, J. Crystal Growth 243 (2002), 243-260.



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

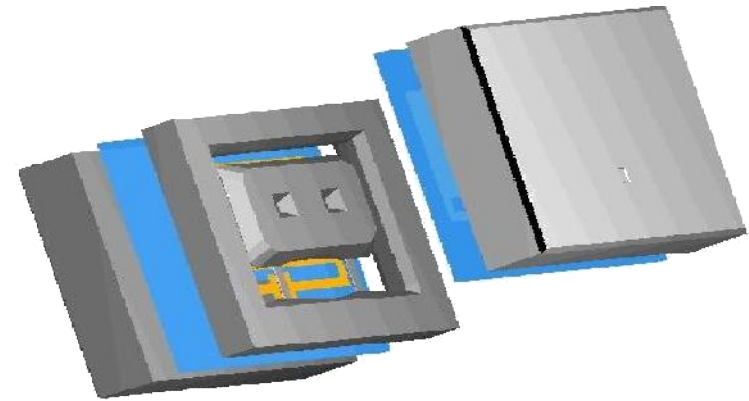
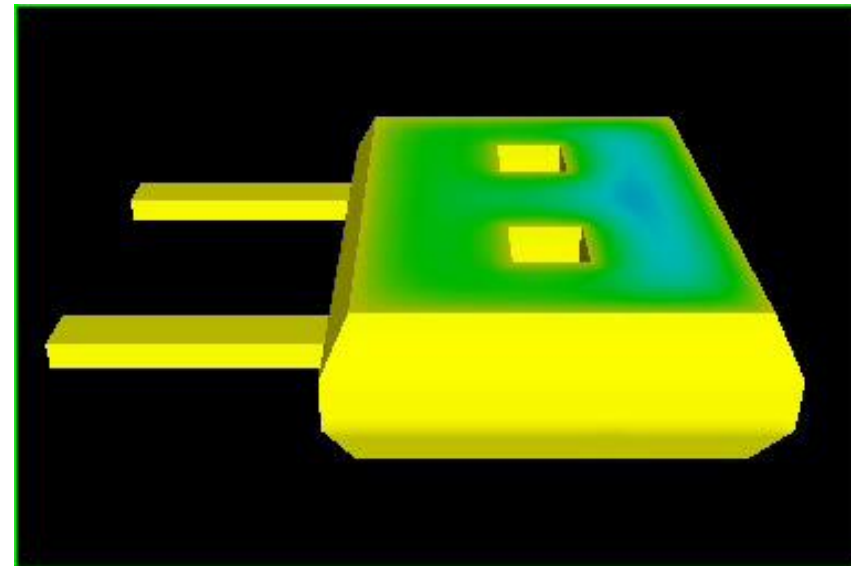
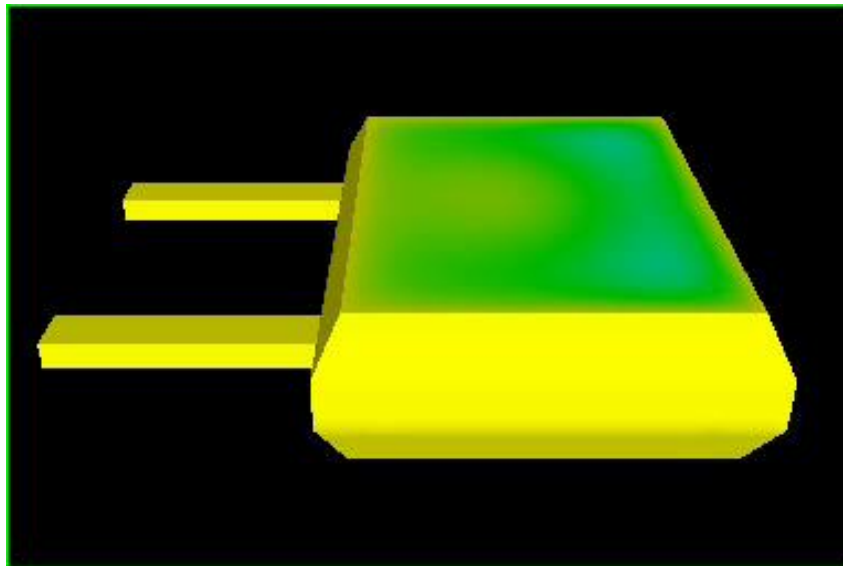
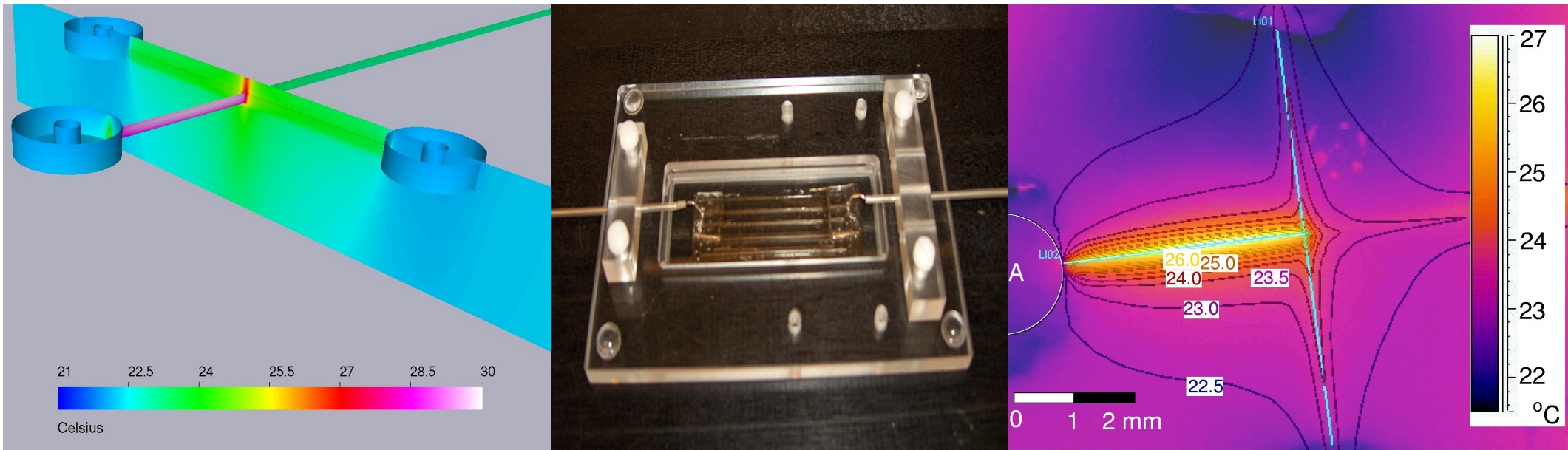


Figure by VTI Technologies

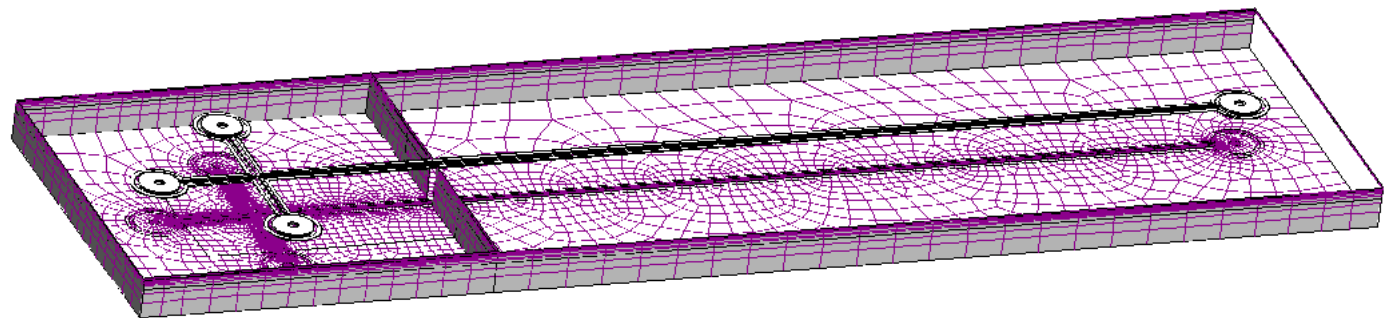


A. Pursula, P. Råback, S. Lähteenmäki and J. Lahdenperä, *Coupled FEM simulations of accelerometers including nonlinear gas damping with comparison to measurements*, J. Micromech. Microeng. **16** (2006), 2345-2354.

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**

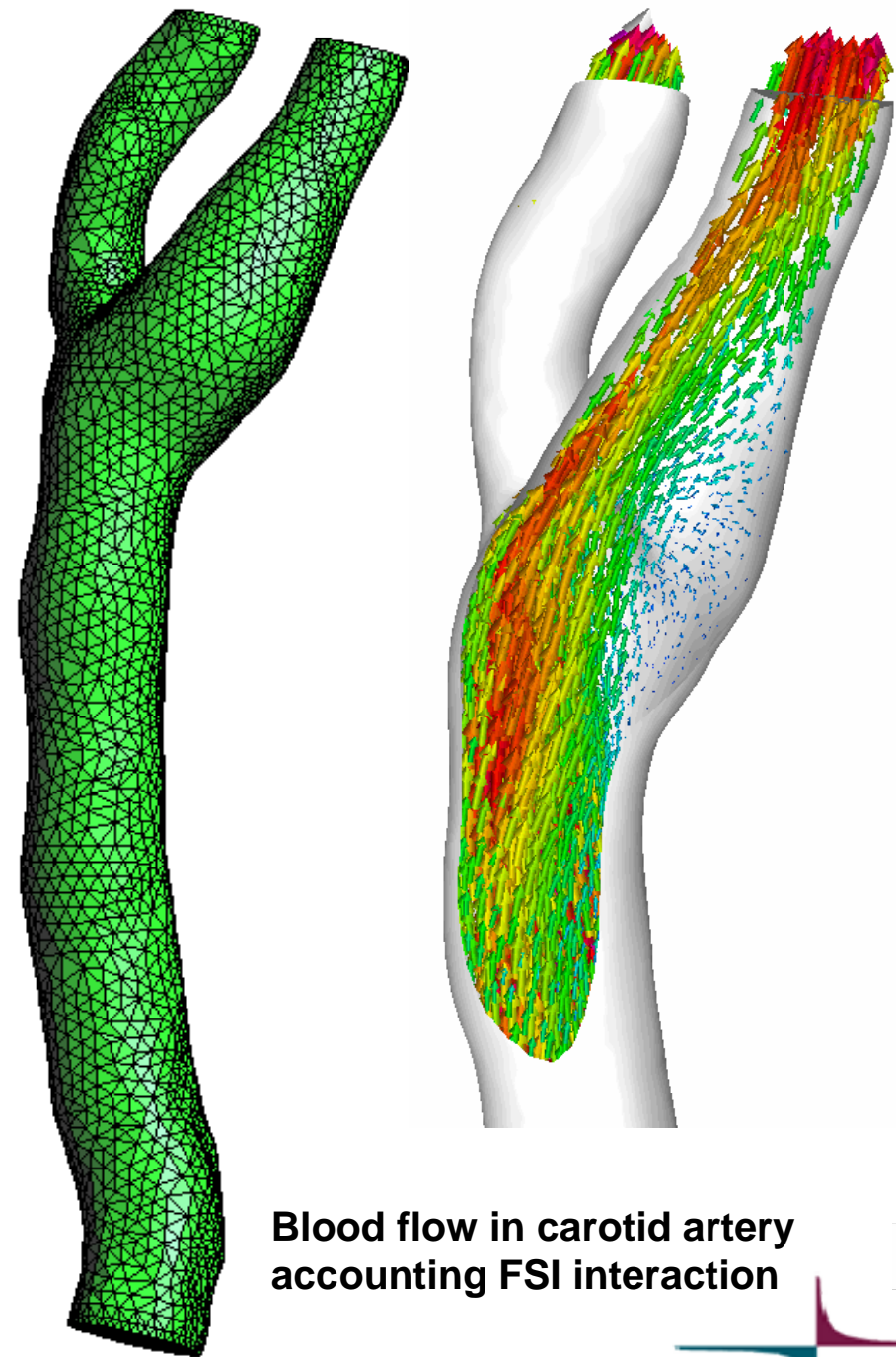


T. Sikanen, T. Zwinger, S. Tuomikoski, S. Franssila, R. Lehtiniemi, C.-M. Fager, T. Kotiaho and A. Pursula, *Microfluidics and Nanofluidics* (2008)

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. Salenius. *A method for partitioned fluid-structure interaction computation of flow in arteries. Medical Eng. & Physics (in press)*

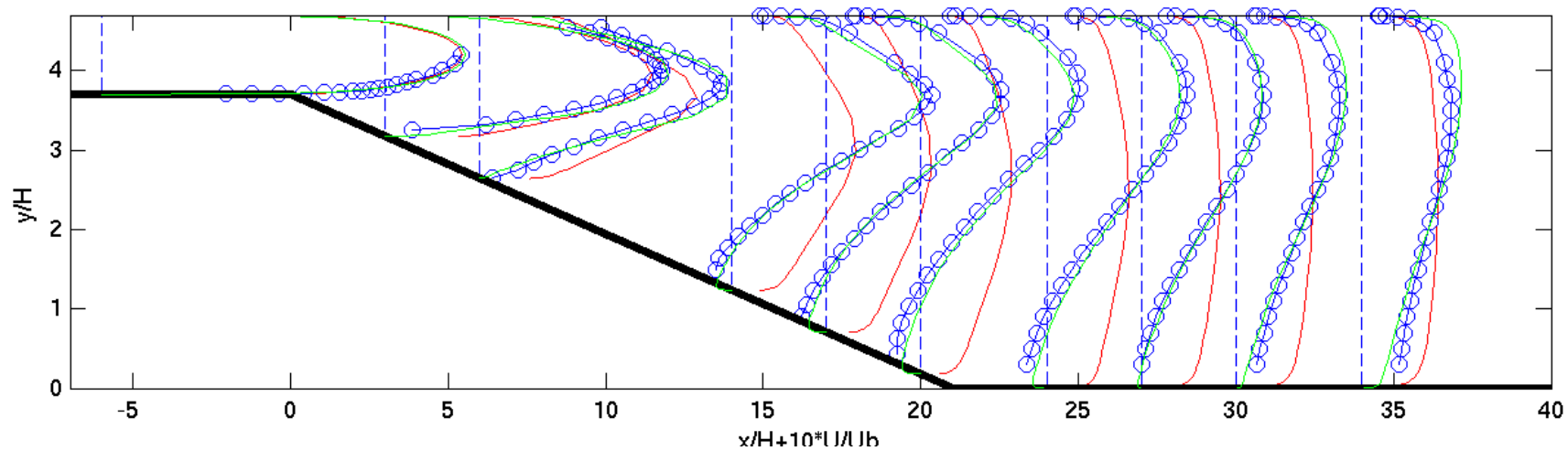


Blood flow in carotid artery accounting FSI interaction

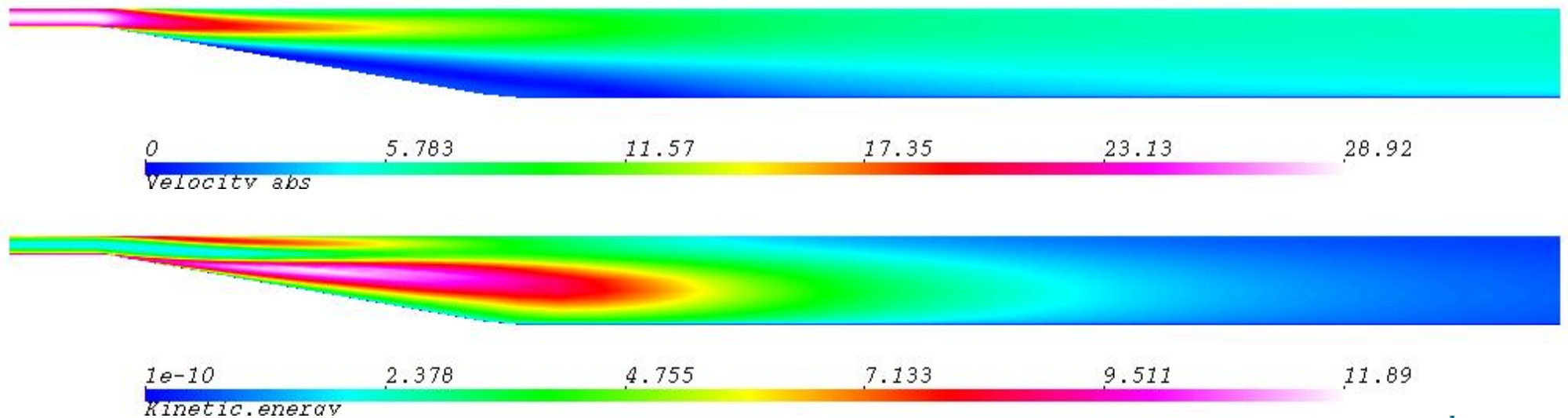


RANS Turbulence modeling

Comparison of $k-\varepsilon$ vs. v^2-f -turbulence models (red & green line)

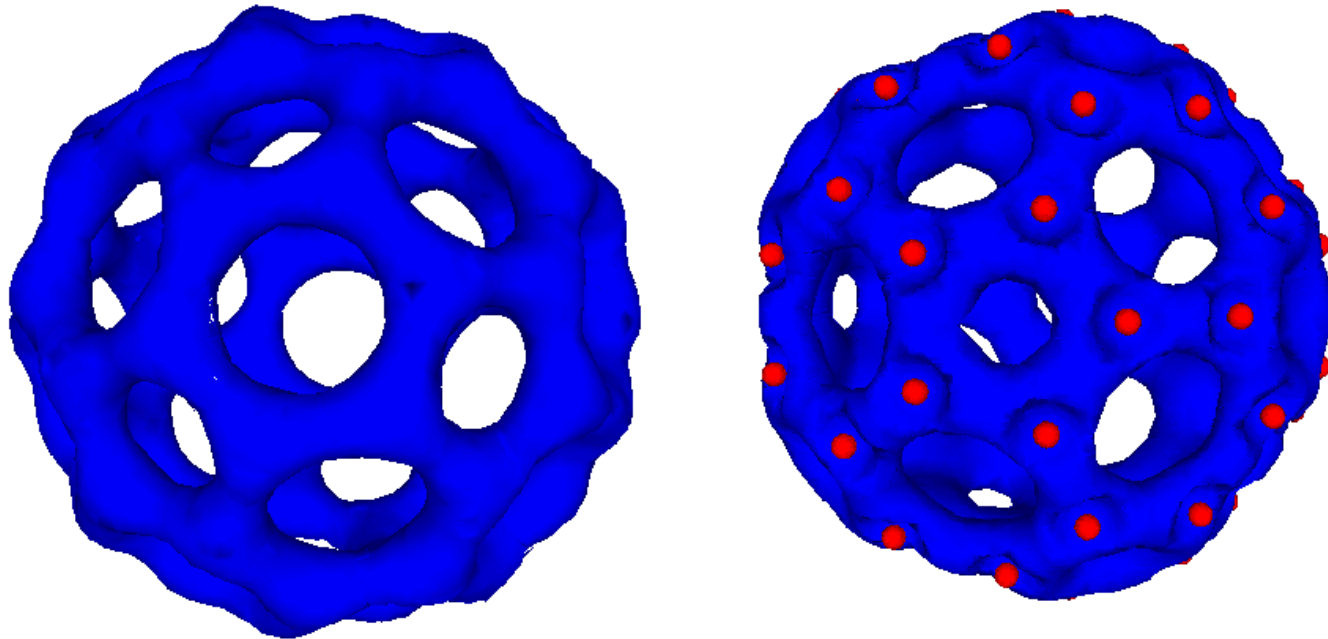


Simulation J. Ruokolainen, CSC



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



Simulation Mikko Lyly, CSC