Elmer Finite Element Software for Multiphysical Optimization Problems

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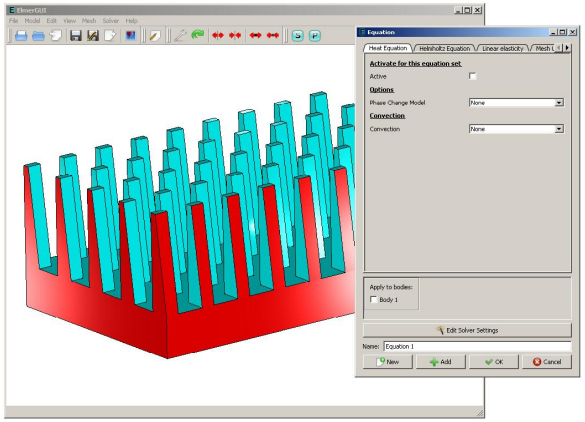
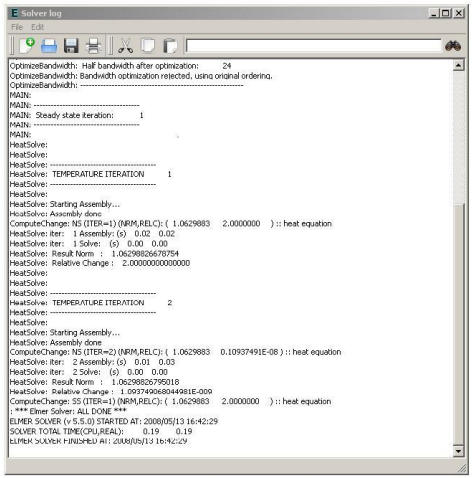
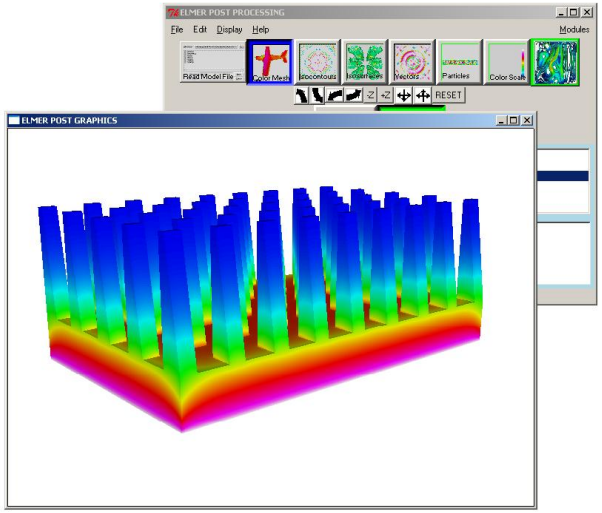
Outline

- Elmer FEM software
- Multiphysical features of Elmer
  - Examples
- Performing optimization with Elmer

Elmer – A finite element software for multiphysical problems







ElmerGUI + ElmerSolver + ElmerPost

ElmerGrid

ElmerFront

CSC

Elmer - Background

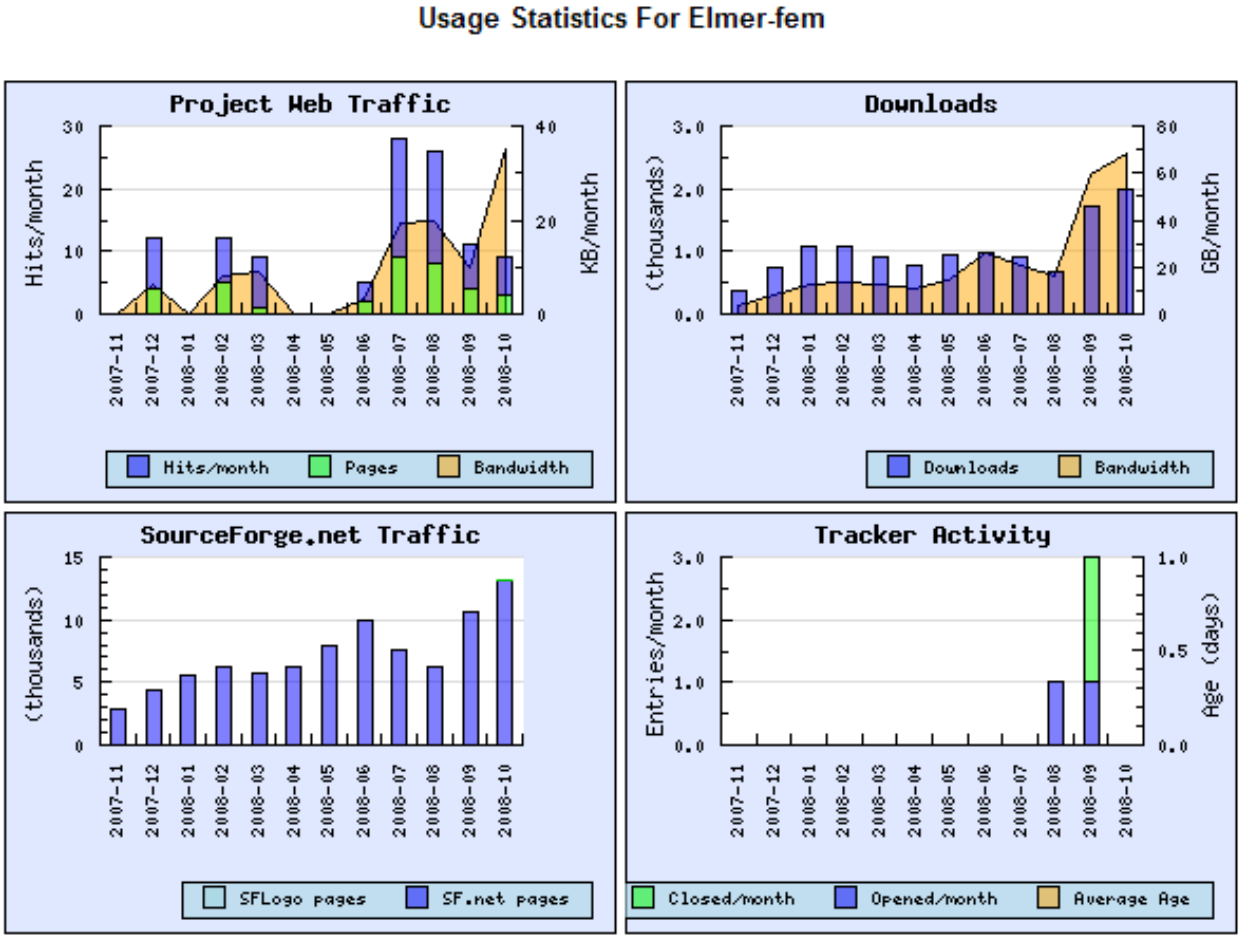
- Solution of partial differential equations by FEM
- Elmer development was started in 1995 as part of a national CFD program, also funded by Tekes
  - Collaboration with TKK, VTT, JyU, and Okmetic Ltd.
- After the initial phase the development has been driven by number of application projects
  - MIKSU (2000-2003) Tekes, VTI Techologies, Vaisala, NRC: MEMS
  - Collaboration with Nokia (2003->): acoustics
  - PIIMA (2004-2005) Tekes & silicon industry: MEMS, microfluidics, crystal growth
  - LSCFD (2008-) Tekes, Okmetic: Large Scale CFD
  - Others: composite structures, optical fiber manufacturing, crystal growth, blood flow, glaciology
  - Computational glaciology: international collaboration
  - Number of thesis projects in universities
- Elmer includes a large number of physical models and modern numerical methods

Elmer goes Open Source

- 9/2005 Elmer published under GPL-license
- 10/2007 Elmer version control put under sourceforce.net
- Goals of the open source publication
  - Expand the Elmer community
  - New resources for code development
  - Improved verification process
  - No resources for a commercial spin-off
  - Free software good adverticiment for CSC
- Roughly 300 000 lines of code!
  - The whole IP of the software still owned by CSC
- Available at
  `http://www.csc.fi/elmer`
  `http://sourceforge.net/projects/elmerfem`

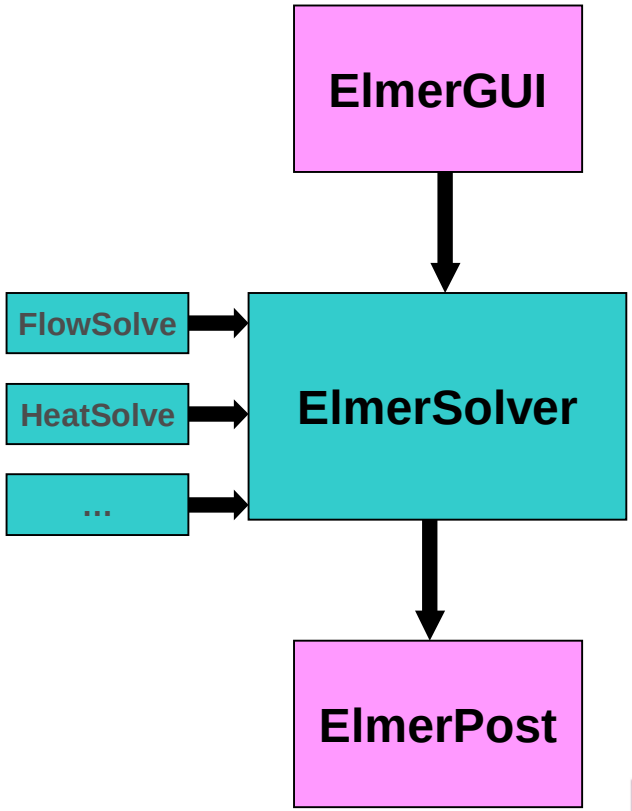
Elmer @sf

- Rank
  ~500
- Downloads
  ~2000 / month



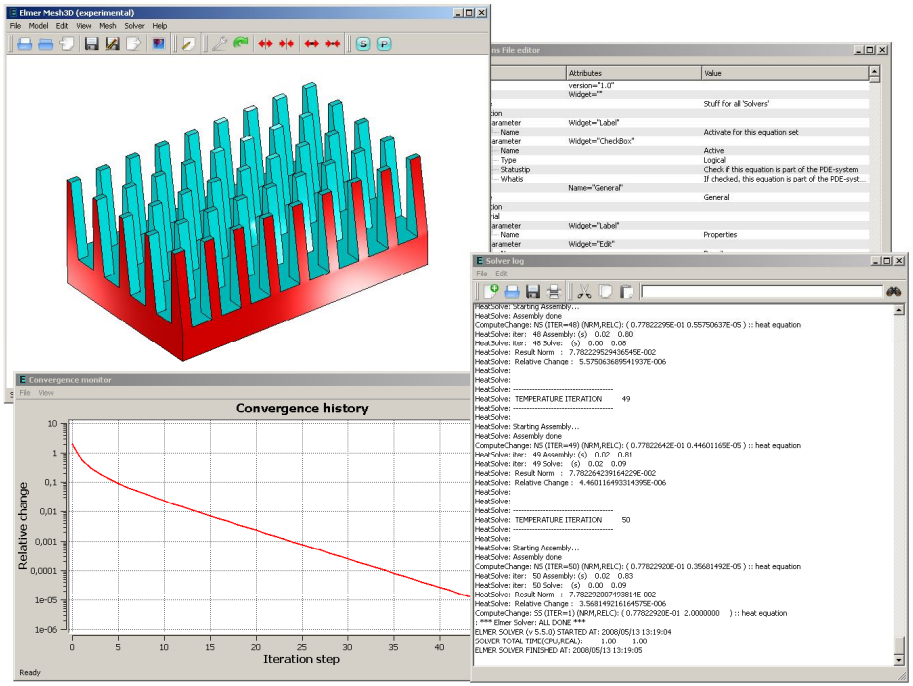
Components of Elmer software suite

- Elmer is actually a suite of several programs
- You may use many of the components independently
- ElmerGUI – Pre- and Postprocessing
- ElmerSolver - Solution
- ElmerPost - Postprocessing
- 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 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
```

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
  - 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
  - Electrostatics & harmonics
  - Magneticstatics
- Electrokinetics
  - Poisson-Boltzmann
  - Poisson-Nernst-Planck
- Quantum mechanics
  - DFT (Kohn Scham)
- ....

Elmer – Numerical Methods

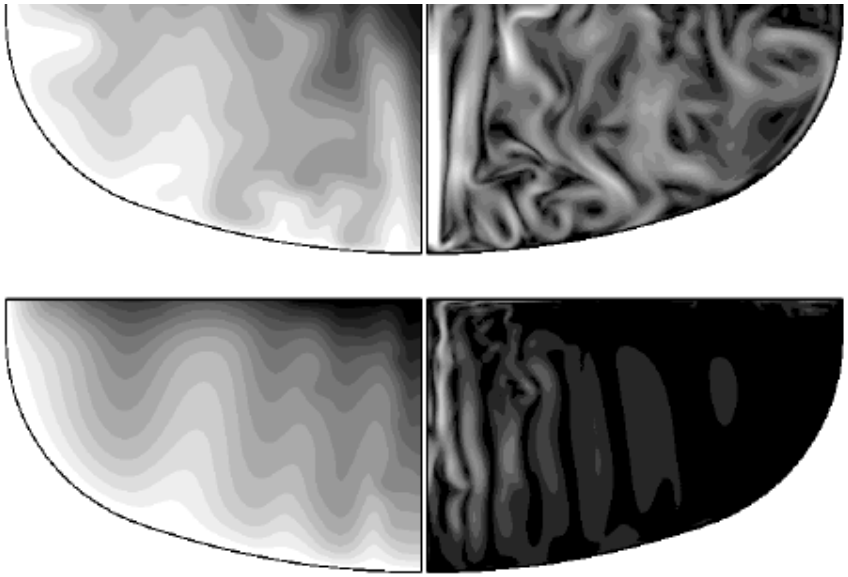
- Time-dependency
  - Static, transient, eigenmode, harmonic, scanning
- Discretization
  - Galerkin, Discontinous Galerkin (DG)
  - Stabilization: SUPG, bubbles
  - Lagrange, edge, face, and p-elements
- Matrix equation solvers
  - Direct: Lapack, Umfpack, (SuperLU, Mumps, Pardiso)
  - Iterative Krylov space methods (own & Hypre)
  - multigrid solvers (GMG & AMG) for “easy” equations (own & Hypre)
  - Preconditioners: ILU, Parasails, multigrid, SGS, Jacobi,...
- Parallellism
  - Parallel assembly and solution (vector-matrix product)
- Adaptivity
  - For selected equations, works well in 2D

Elmer - Multiphysics capabilities

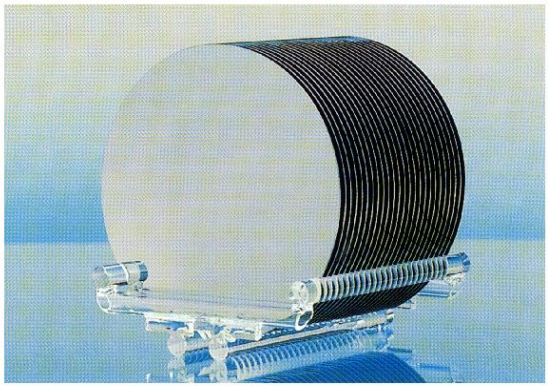
- About 20 different physical models
- Iteration method is mainly used
  - Consistancy of solution is ensured by nested iterations
- Monolithic approach is used for some inherently coupled problems
  - Linearized time-harmonic Navier-Stokes
- For some special problems using iterative coupling convergence 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

Czockralski Crystal Growth

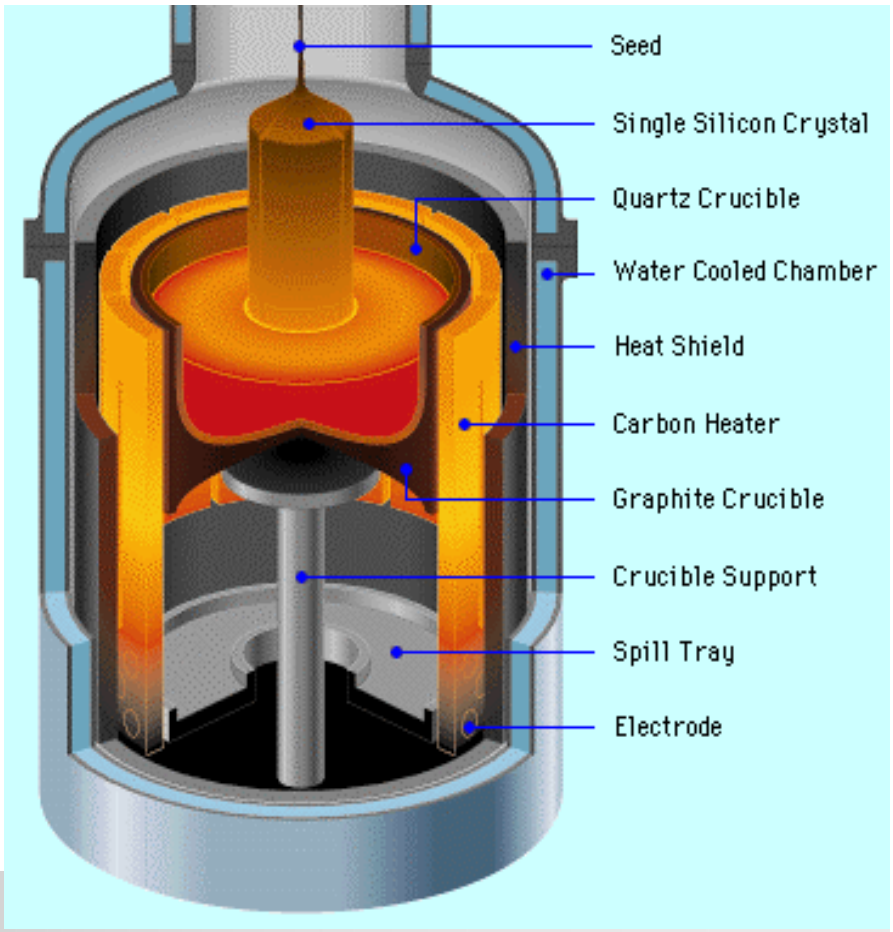
- Most crystalline silicon is grown by the Czhockralski (CZ) method
- One of the key application when Elmer development was started in 1995



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



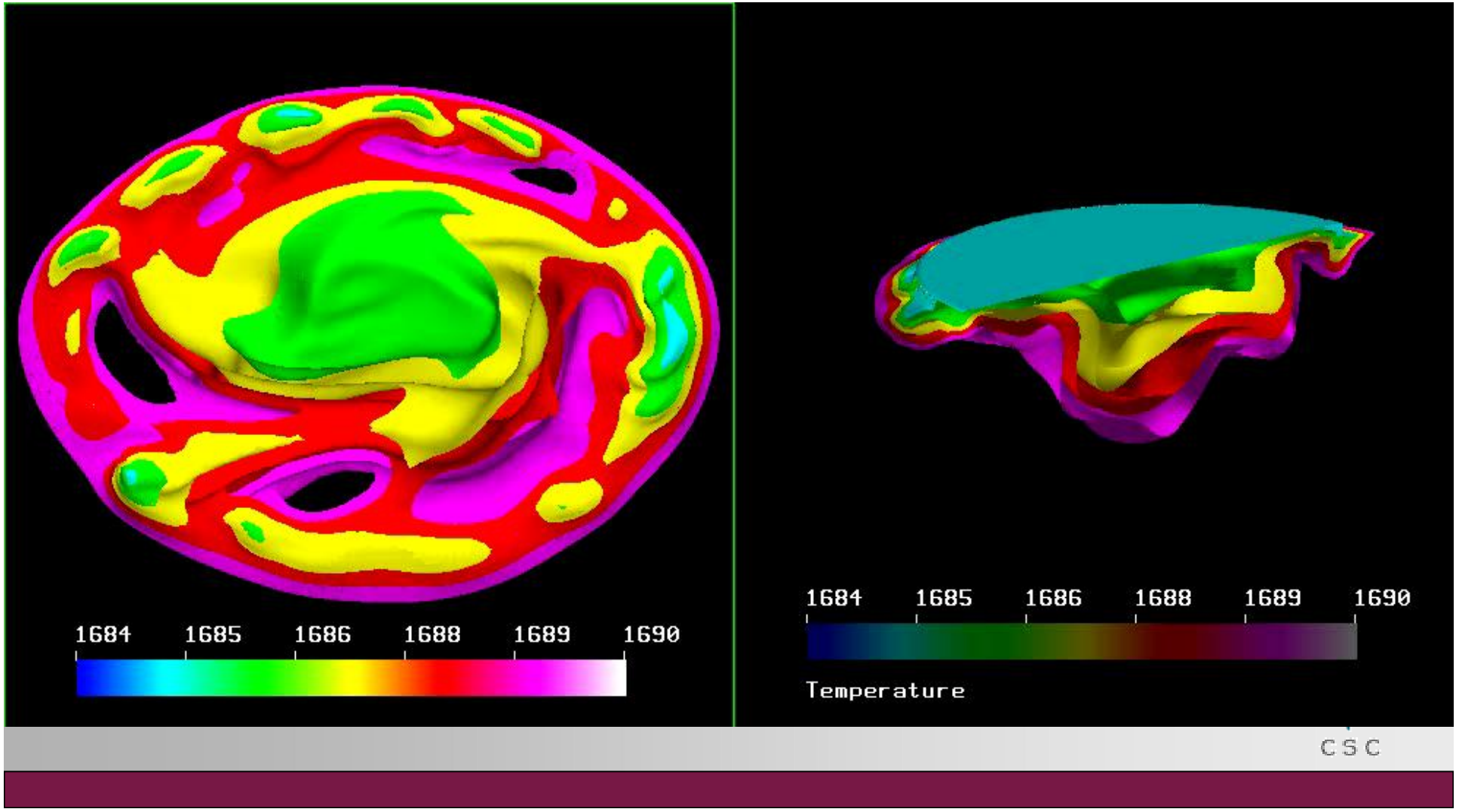
Figures by Okmetic Ltd.



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

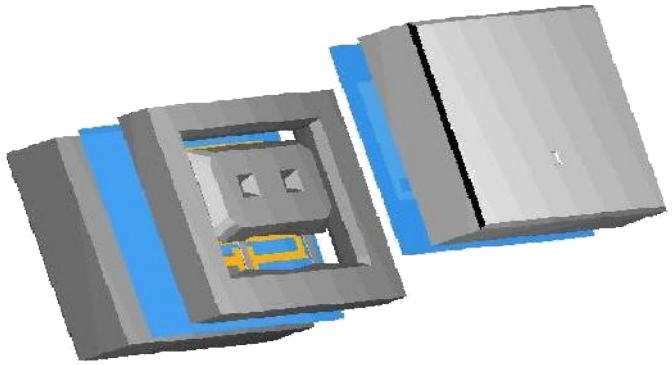
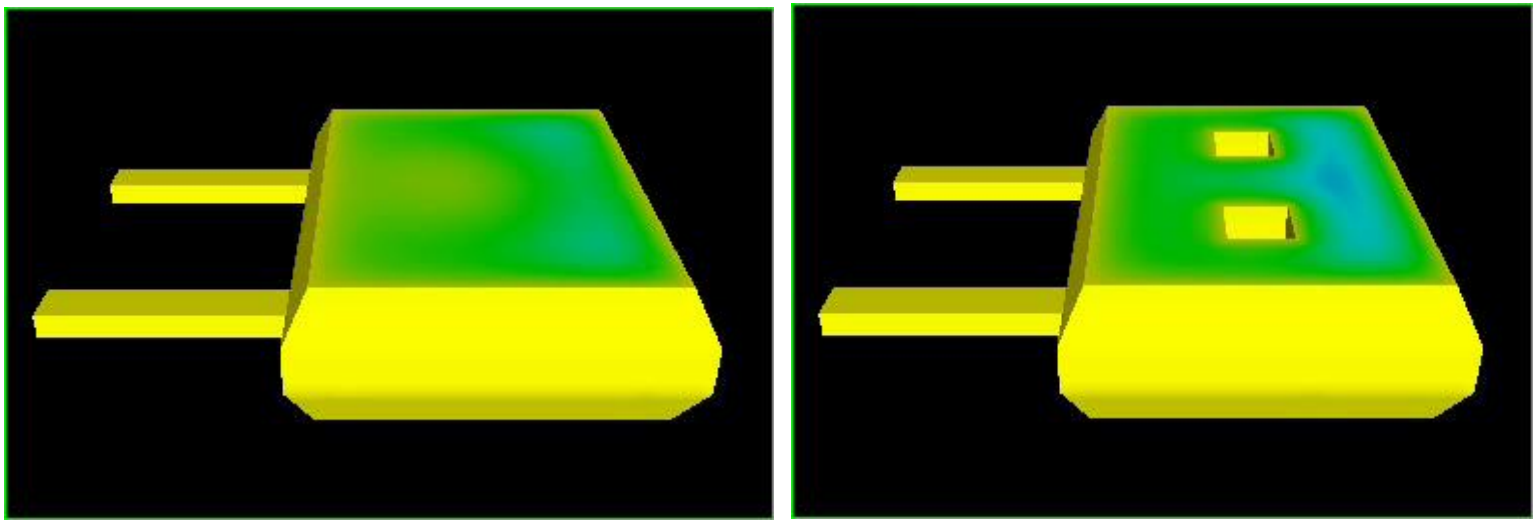


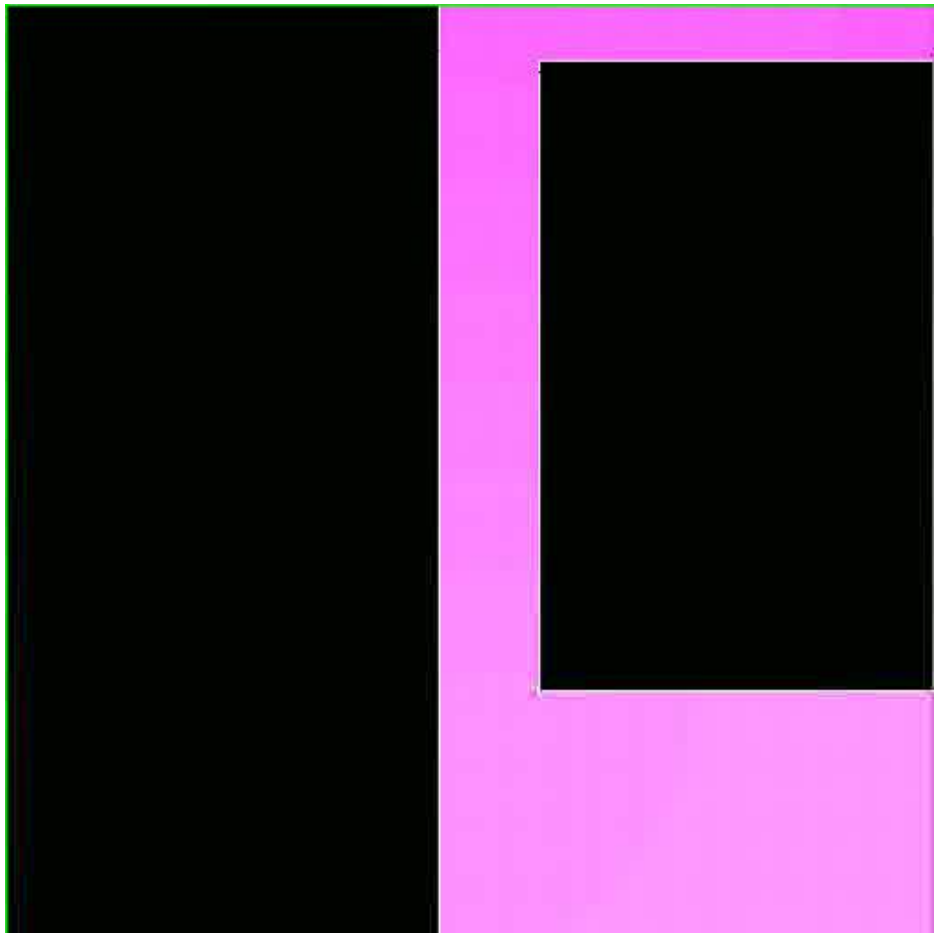
Figure by VTI Technologies



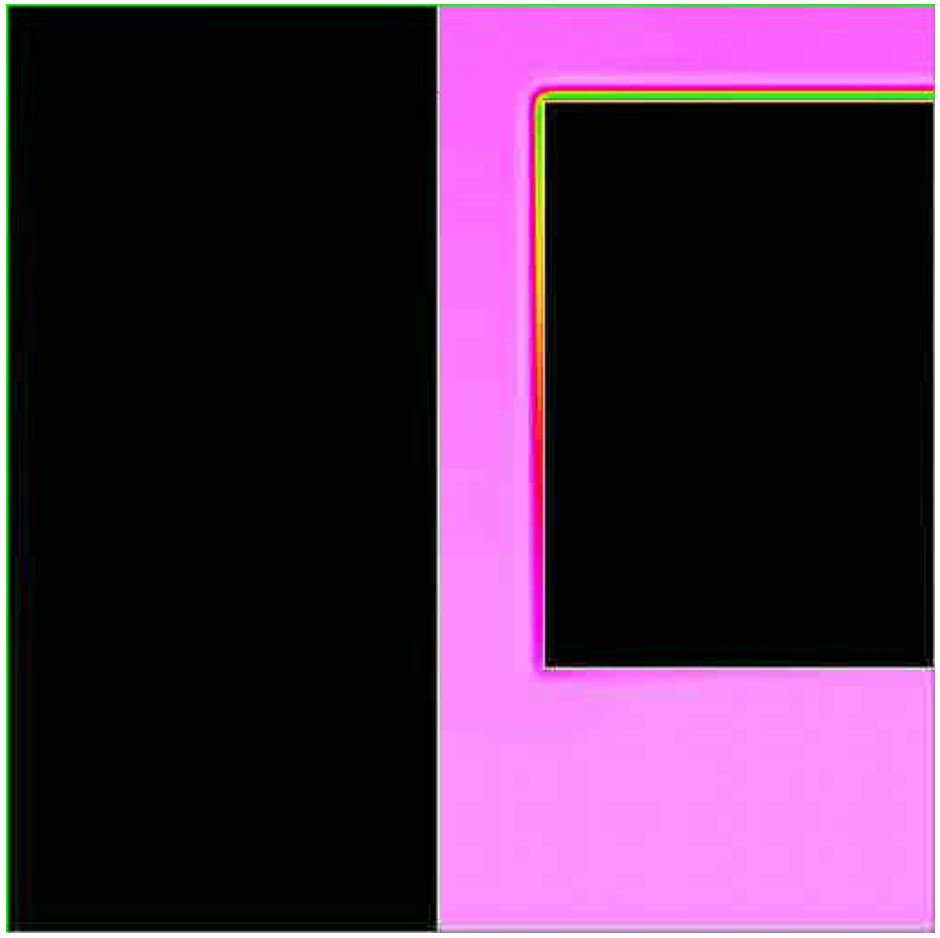
A. Pursula, P. Råback, S. Lähteenmäki and J. Lahdenperä, *Coupled FEM simulations of accelerometers including nonlinear gas damping with comparison to measurements*, J. Micromech. Microeng. **16** (2006), 2345-2354.

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)

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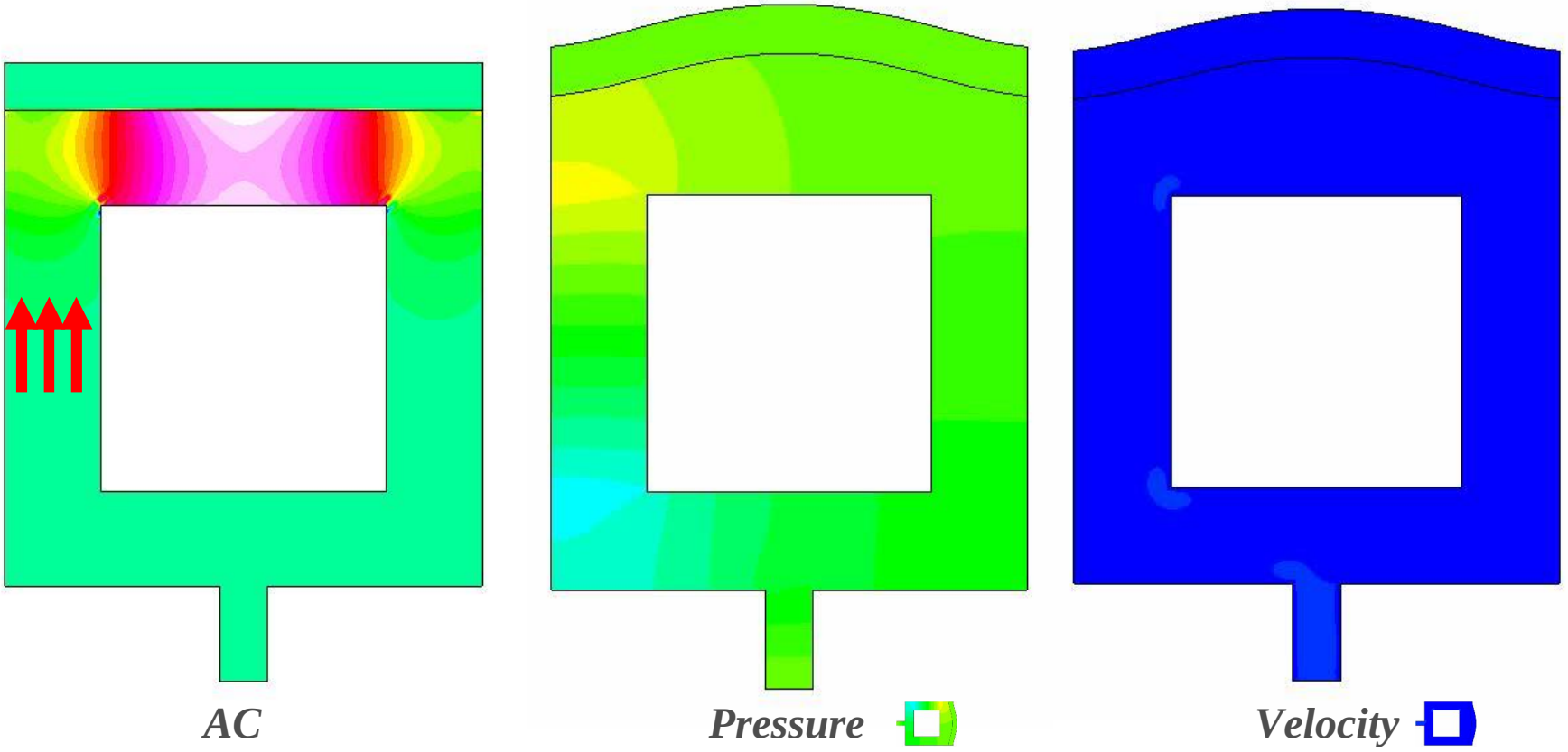
FSI with articifical compressibility

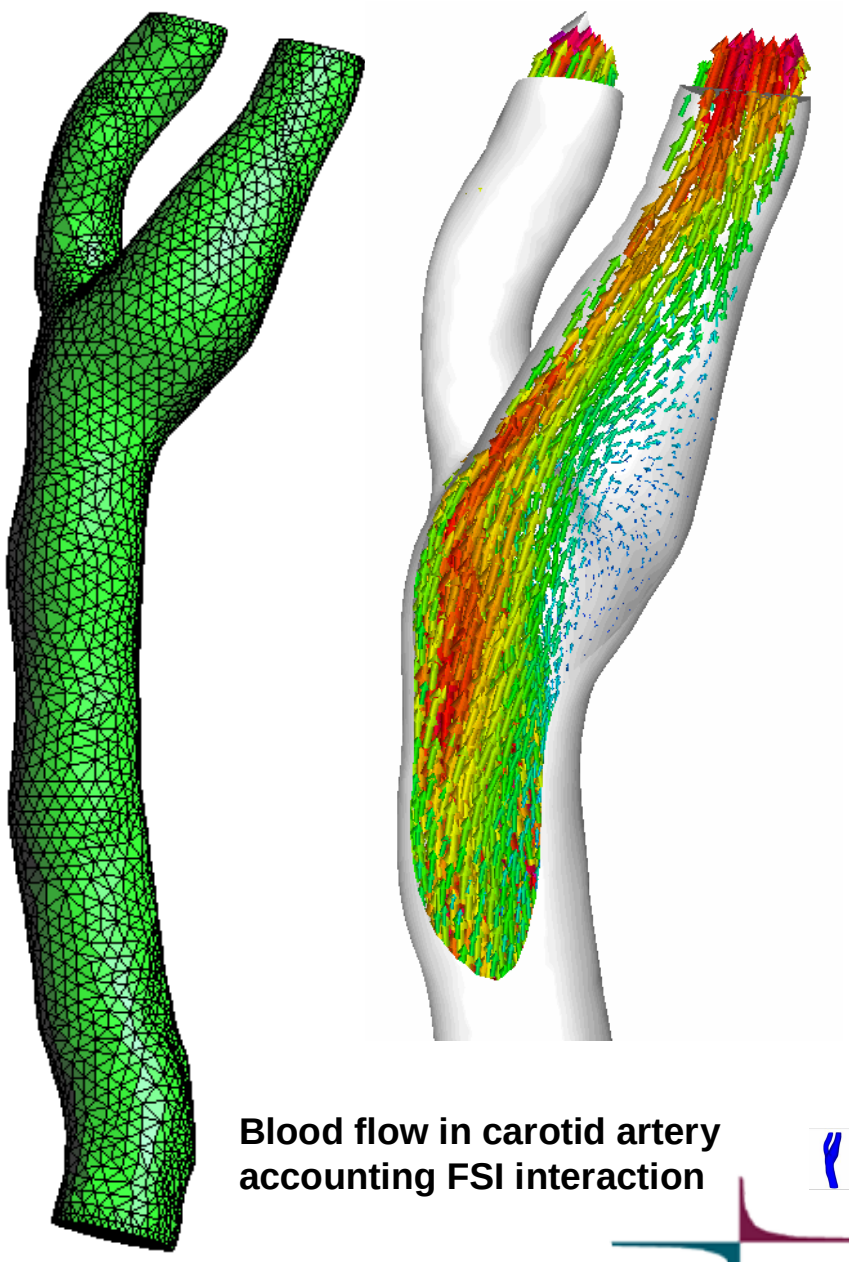
- Flow is initiated by a constant body force at the left channel
- Natural boundary condition is used to allow change in mass balance
- An optinmal artificial compressibility field is used to speed up the convergence of loosely coupled FSI iteration



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

Computational Hemodynamics

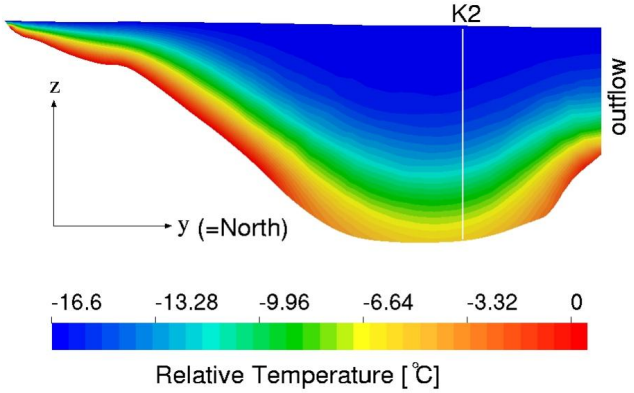
- Cardiovascular diseases are the leading cause of deaths in western countries
- Calcification reduces elasticity of arteries
- Modeling of blood flow poses a challenging case of fluid-structure-interaction
- Artificial compressibility is used to enhance the convergence of FSI coupling

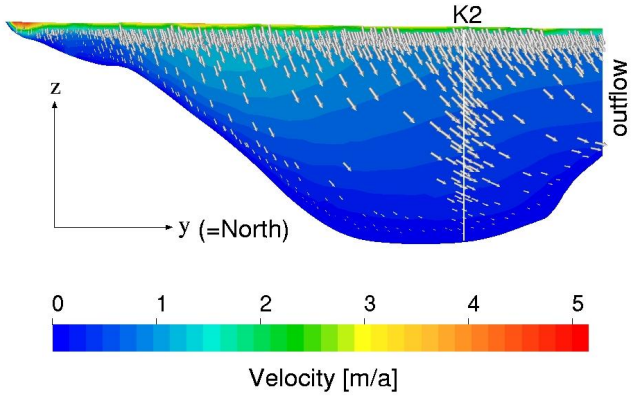


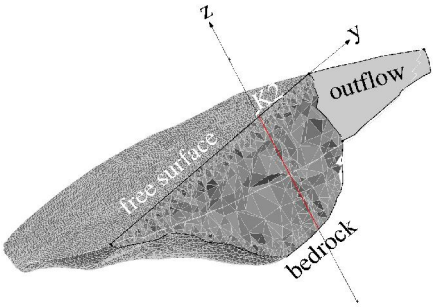
Blood flow in carotid artery accounting FSI interaction

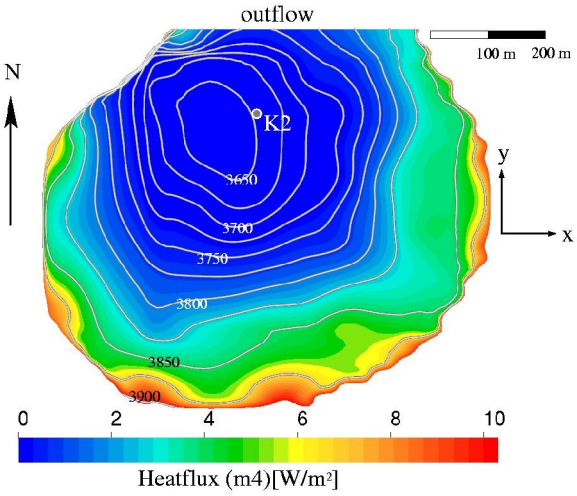
E. Järvinen, P. Råback, M. Lyly, J. Salonius. *A method for partitioned fluid-structure interaction computation of flow in arteries. Medical Eng. & Physics*, **30** (2008), 917-923

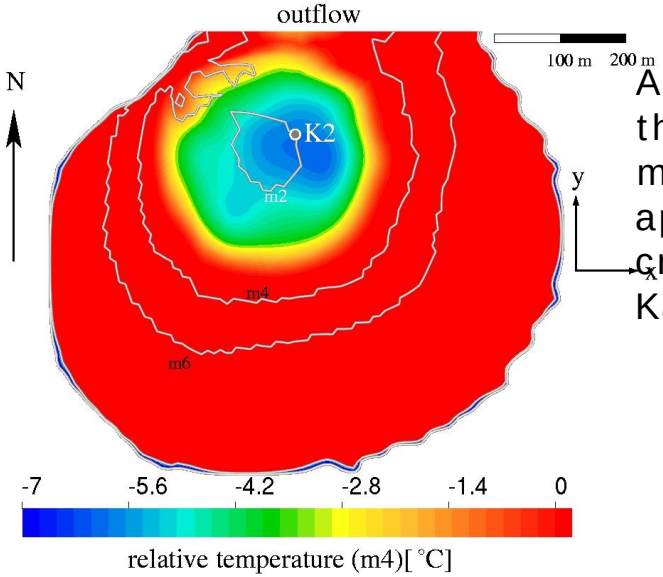
Glaciology: 3D Stokes of glaciers











A full Stokes-flow thermo-mechanical model for firn and ice applied to the Gorshkov crater glacier, Kamchatka

Zwinger, Greve, Gagliardini, Shiraiwa and Lyly
Annals of Glaciology 45 (2007)

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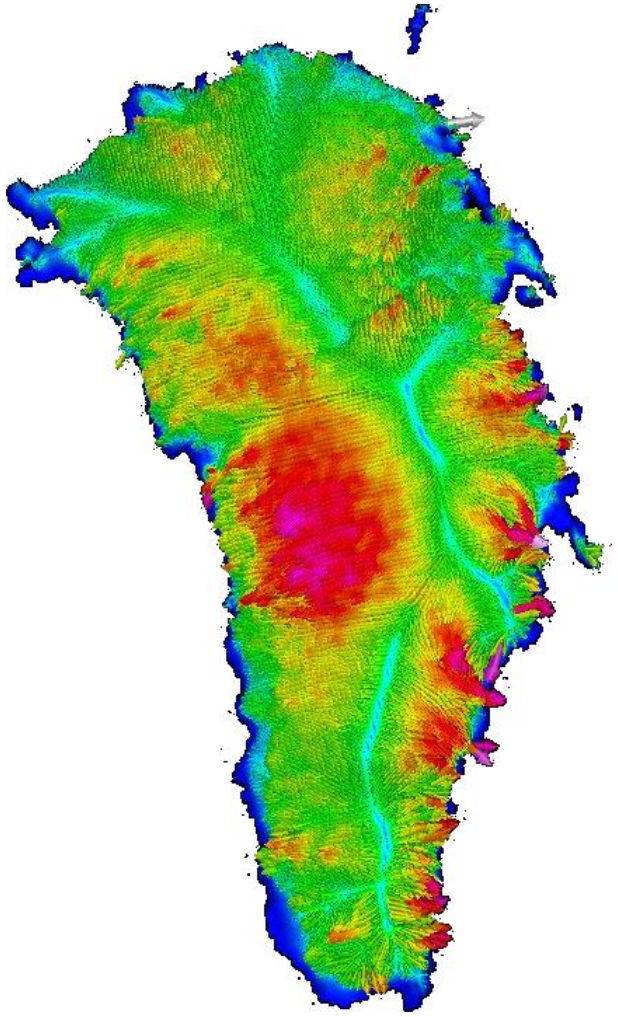
Glaciology: Grand challenges

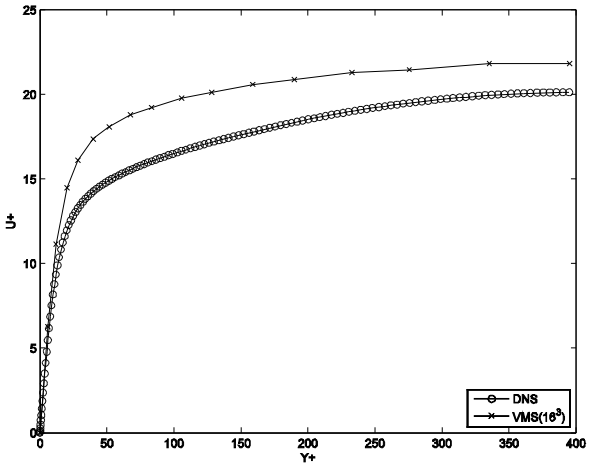
- Elmer uses full Stokes equation to model the flow of ice
- Currently the mostly used tool in the area
  - British Antarctic Survey
  - University of Grenoble
  - University of Sapporo
- Simulations of continental ice sheets very demanding
- Global warming makes the simulations very important



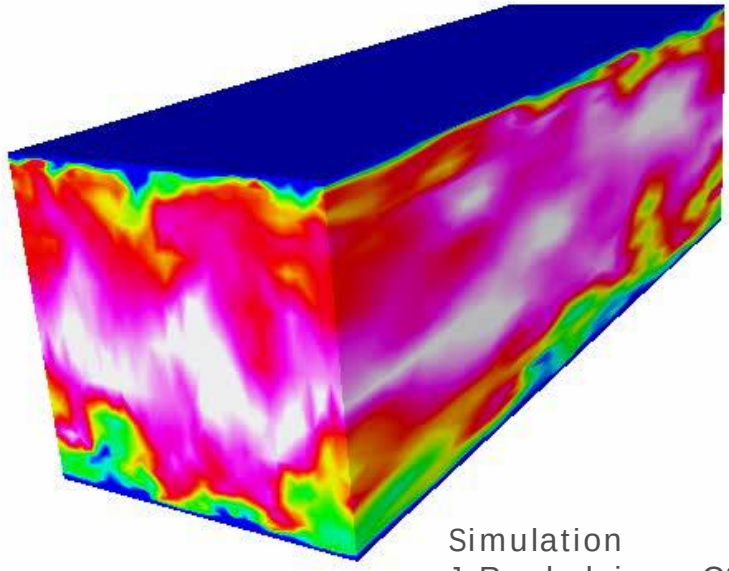
Simulation T. Zwinger, CSC

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 using 16^3 quadratic mesh

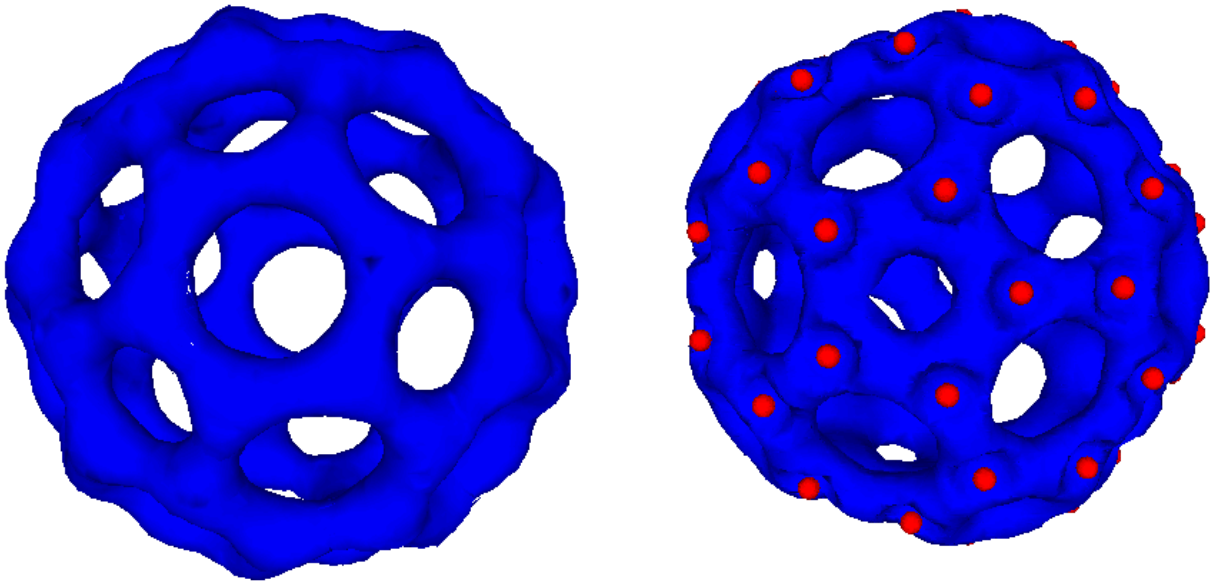


Simulation
J. Ruokolainen, CSC

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



Simulation Mikko Lyly, CSC

Optimization and Elmer

- Optimization hasn't been a major theme in the development of Elmer
- Several applications over the years
  - Optimization in FSI within a Tekes funded project in 2001 using Synaps Pointer (later known as Epogy)
  - Optimization of composite structures with GRIDs (P. Kere et al.)
  - Structural opptimization (J. Mäkipelto et.al.)
  - ...
- Most applications have implemented their own interfaces but there are also some tools to help in the optimization
  - FindOptimum solver (dll of ElmerSolver)
  - ElmerParam interface (independent)

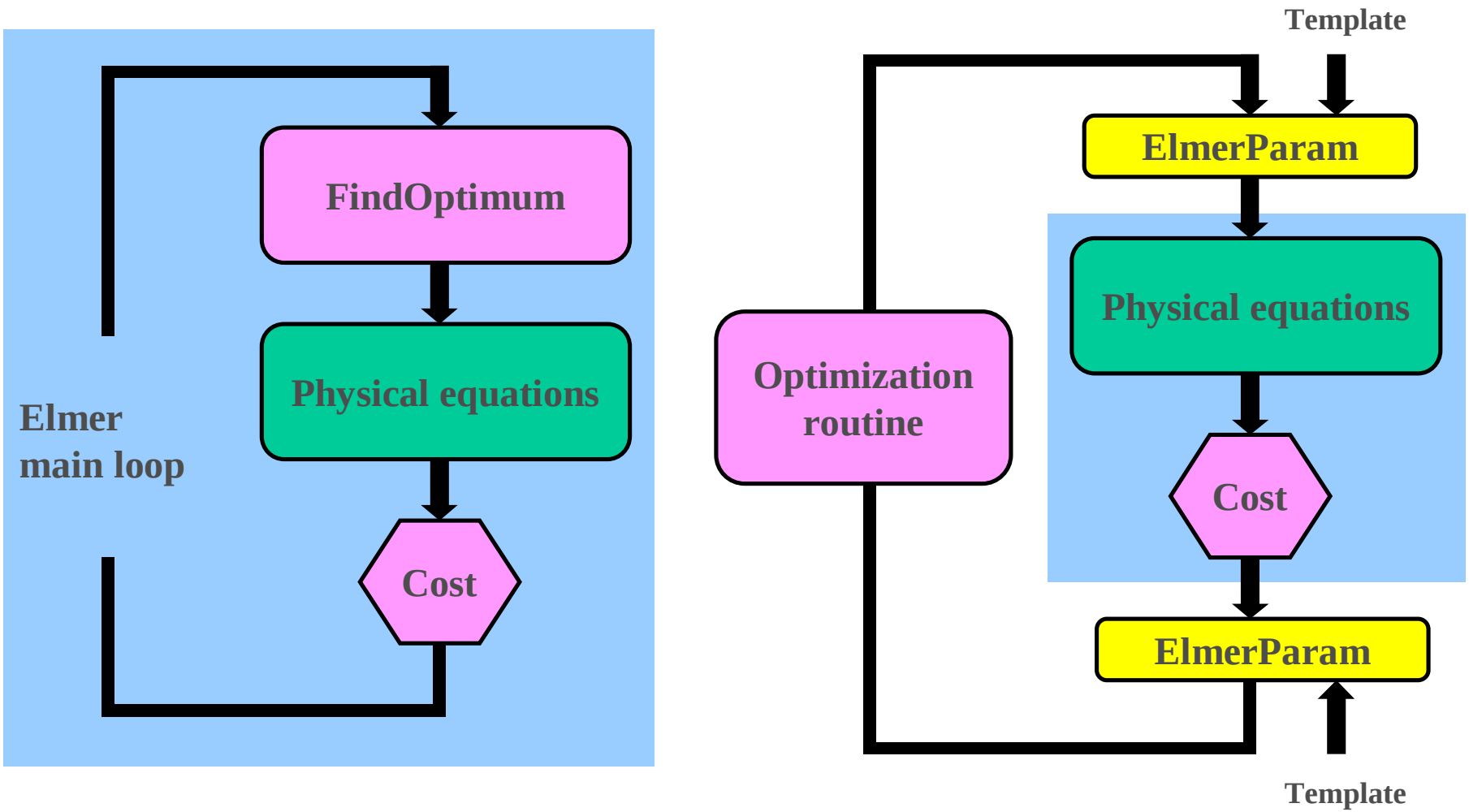
FindOptimum solver

- A normal solver of Elmer that uses different strategies for modifying design parameters
  - Simplex
  - Genetic optimization
  - ...
- The material properties or geometric deformations may depend on these parameters
- Does not have a ruling position in the workflow
  - Elmer main program not affected
  - Often requires rewriting of the optimization algorithms
- Does not require reinitialization of the FE job
  - Preferable if no remeshing needed
  - Optimal performance

ElmerParam package

- Small C library
- Provides optimization wrapper around any code that uses ascii input and output
  - Create template files for input files
    input.dat -> input.dat.model
  - <!Pn!> replaced by n:th parameter value
    <!P1!> -> 0.123
- Does not include any optimization algorithms itself
- The optimization algorithms may call Elmer as a black-box function to evaluate the cost functions
  - Provides f90 and C functions for blackbox optimizations
  - Includes also interfaces for Matlab (mex), APPSPACK, and R
  - No need to rewrite any algorithms
- Not limited just to the Elmer package
- Supports also integer and mixed parameters

FindOptimum vs. ElmerParam



Remarks on optimization

- Elmer has been previously used with Epogy and there its should be easy to any other commercial optimization package
  - modeFRONTIER,...
- Elmer does not include automatic derivation
  - Only black box approach available
- Experience has shown that if the mesh remains constant gradient-based methods often prevail
  - High accuracy requirements on linear and nonlinear system level
- Changing mesh creates unphysical jumps to the cost function
  - Best compatible with GA methods

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
- Peter.Raback@csc.fi

Thank you for your attention!