# Elmer

## Overview of Physical Models with Examples

ElmerTeam

CSC – IT Center for Science Ltd.

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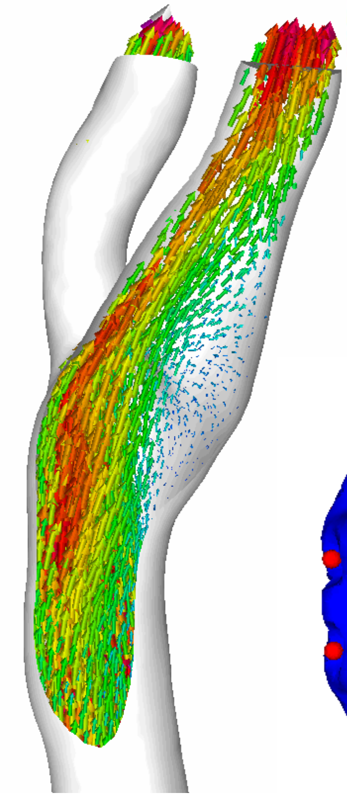
# Elmer – Numerical Methods

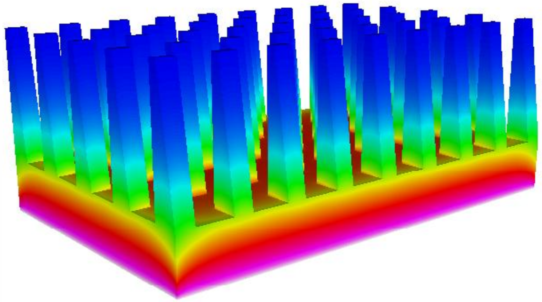
- Time-dependency
  - Static, transient, eigenmode, scanning
- Discretization
  - Element families: nodal, edge, face, and p-elements, DG
  - Formulations: Galerkin, stabilization, bubbles
- Linear system solvers
  - Direct: Lapack, Umfpack, (SuperLU, Mumps, Pardiso)
  - Iterative Krylov space methods (HutIter & Hypre)
  - multigrid solvers (GMG & AMG) for “easy” equations (own & Hypre)
  - Preconditioners: ILU, BILU, Parasails, multigrid, SGS, Jacobi,…
- Parallellism
  - Parallel assembly
  - Solution with selected methods
- Adaptivity
  - For selected equations, works well in 2D

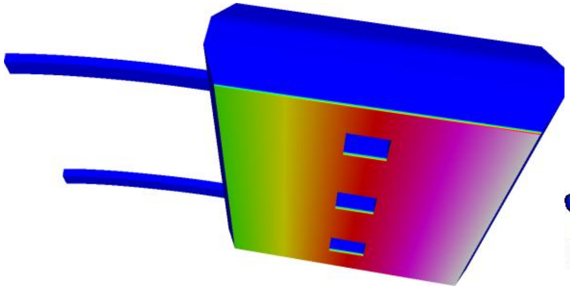
# Elmer - Physical Models

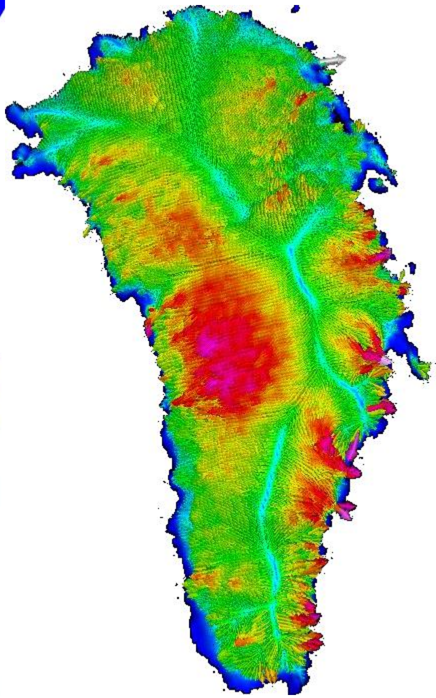
- Heat transfer
  - Heat equation
  - Radiation with view factors
  - convection and phase change
- Fluid mechanics
  - Navier-Stokes (2D & 3D)
  - RANS: *SST* $k$-$\Omega$, $k$-$\varepsilon$, $v^2$-$f$
  - LES: VMS
  - Thin films: Reynolds (1D & 2D)
- Structural mechanics
  - General Elasticity (unisotropic, lin & nonlin)
  - Plate, Shell
- Acoustics
  - Helmholtz
  - Linearized time-harmonic N-S
  - Monolithic thermal N-S
- Species transport
  - Generic convection-diffusion equation
- Electromagnetics
  - Emphasis on steady-state and harmonic analysis
  - New Whitney element formulation for magnetic fields
- Mesh movement (Lagrangian)
  - Extending displacements in free surface problems
  - ALE formulation
- Level set method (Eulerian)
  - Free surface defined by a function
- Electrokinetics
  - Poisson-Boltzmann
- Thermoelectricity
- Quantum mechanics
  - DFT (Kohn Scham)
- Particle Tracker
- ….

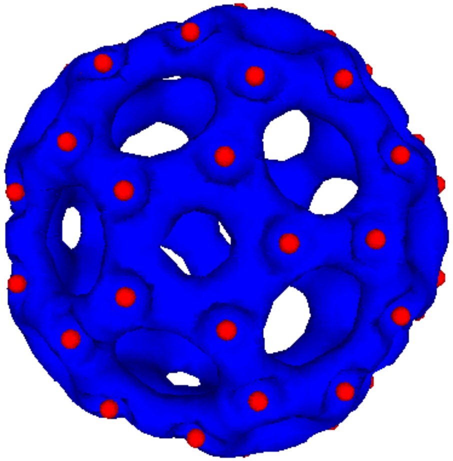
# Elmer Simulations

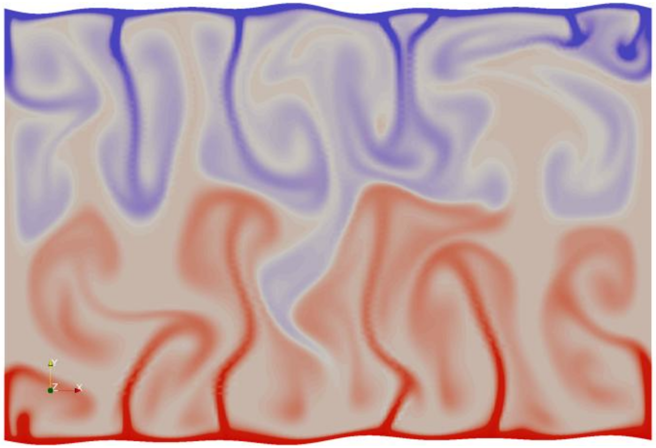


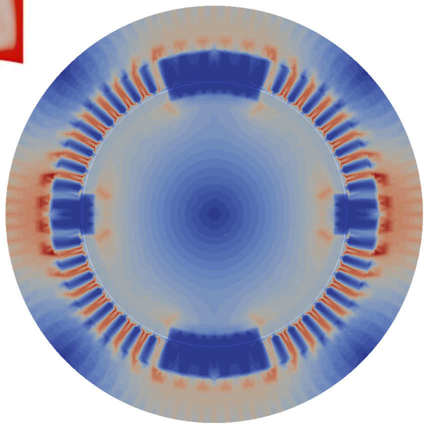


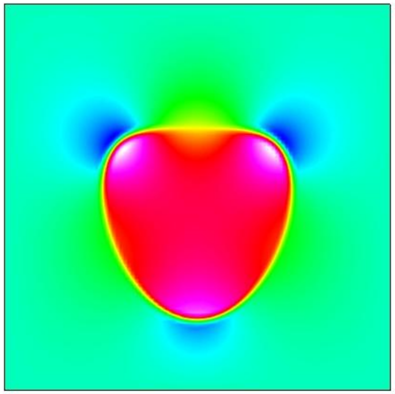


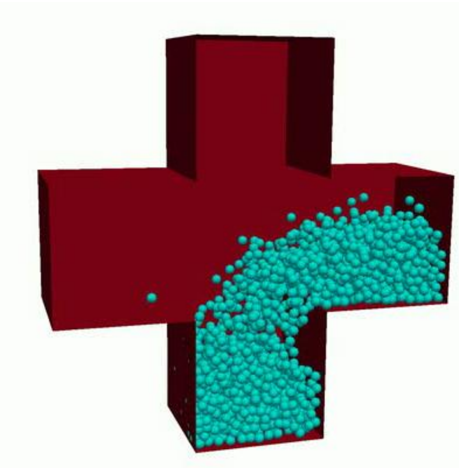


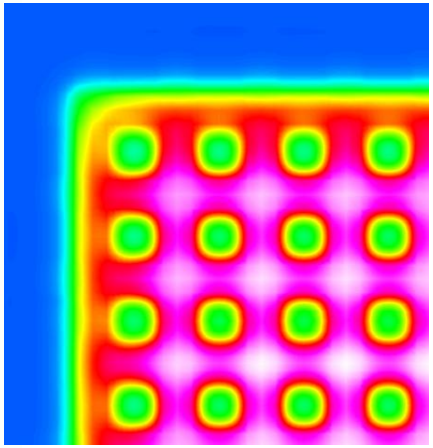






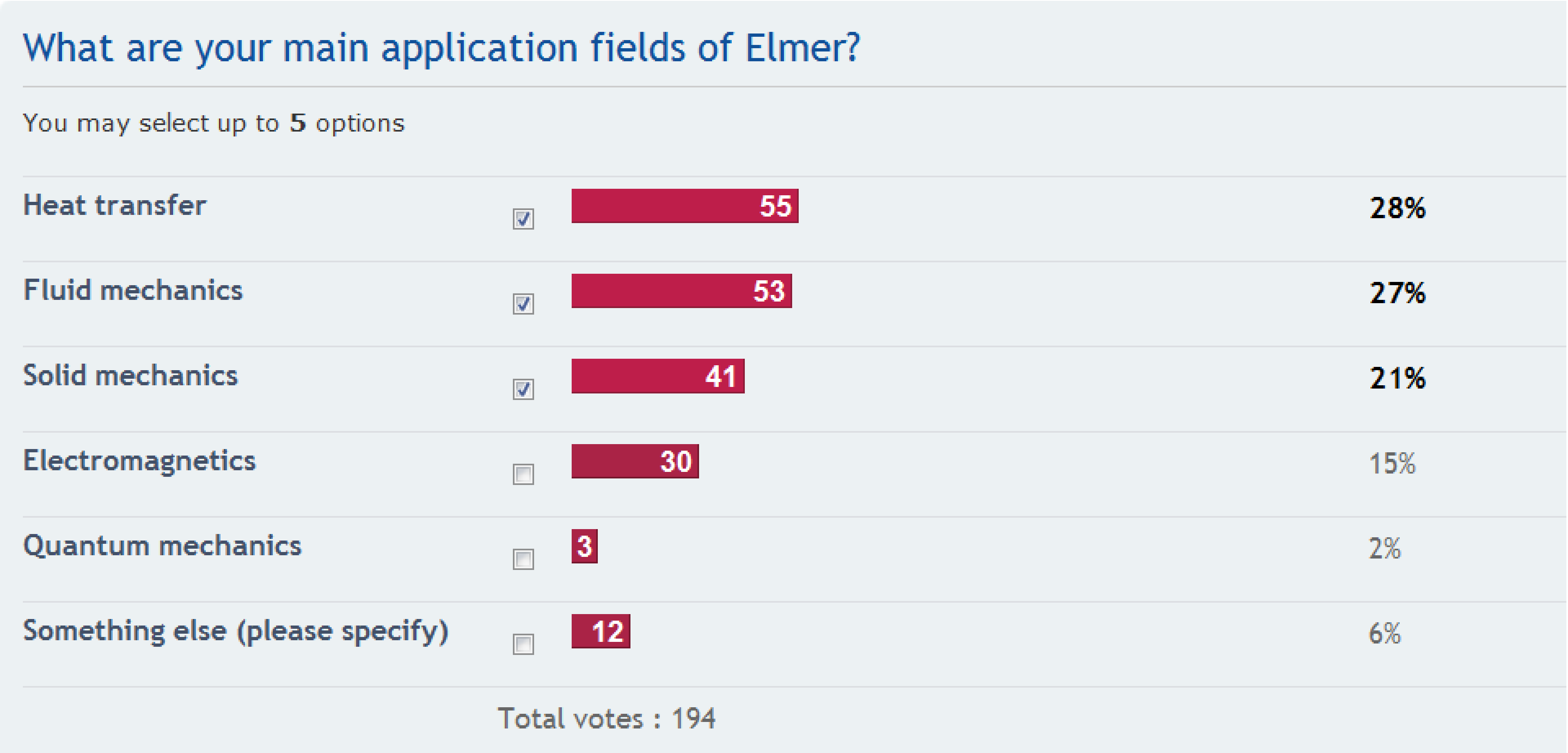






Figures by Esko Järvinen, Mikko Lyly, Peter Råback, Timo Veijola (TKK) & Thomas Zwinger

# Application Fields – Poll (Status 10/2012)



## What are your main application fields of Elmer?

You may select up to **5** options

| | | | |
|---|---|---|---|
| Heat transfer | ☑ | 55 | **28%** |
| Fluid mechanics | ☑ | 53 | **27%** |
| Solid mechanics | ☑ | 41 | **21%** |
| Electromagnetics | ☐ | 30 | 15% |
| Quantum mechanics | ☐ | 3 | 2% |
| Something else (please specify) | ☐ | 12 | 6% |

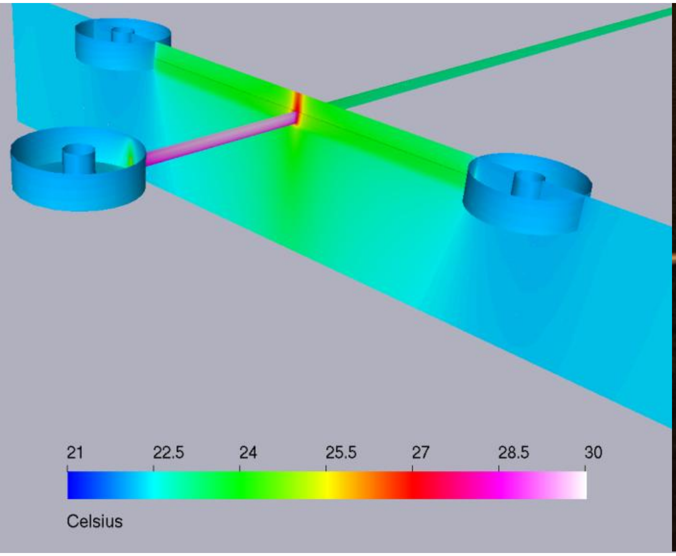
Total votes : 194

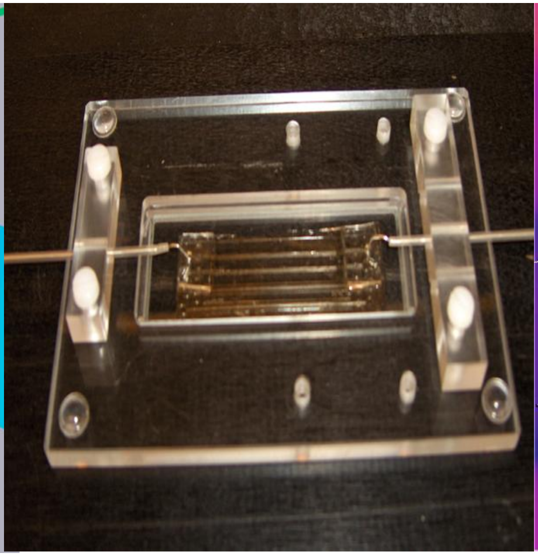
# Elmer – Heat Transfer

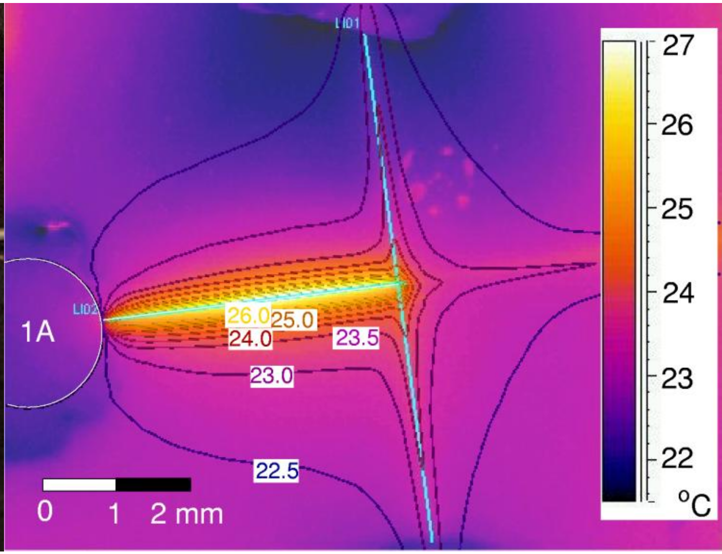
- Heat equation
  - convection
  - diffusion
  - Phase change
  - Temperature control feedback
  - Thermal slip BCs for small Kn number
- Radiation with view factors
  - 2D, axisymmetric use numerical integration
  - 3D based on ray tracing
  - Stand-alone program
- Strongly coupled thermoelectric equation

- 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

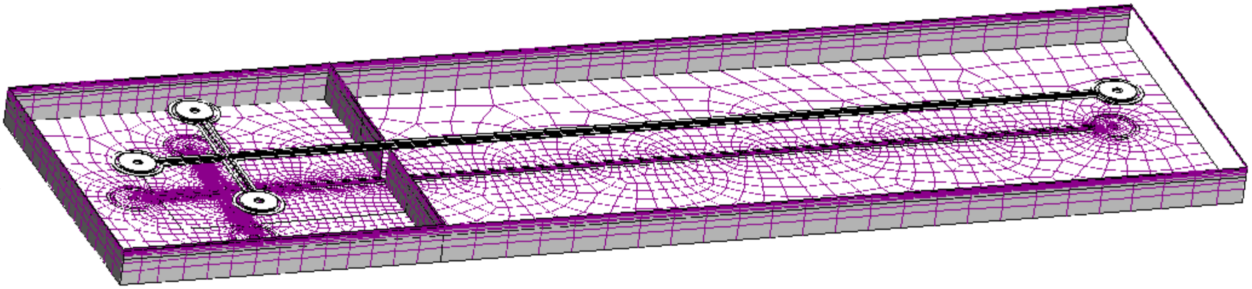
# Microfluidics: Flow and heat transfer in a microchip







- 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 – 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

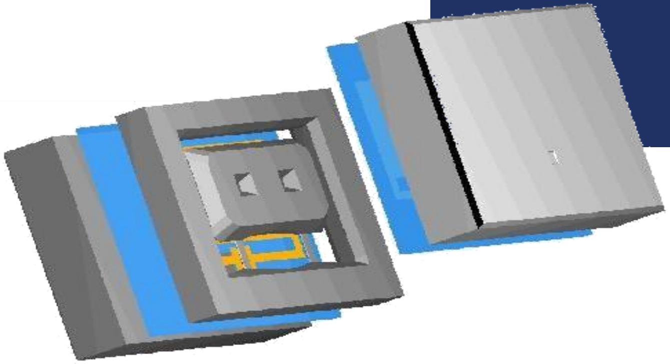
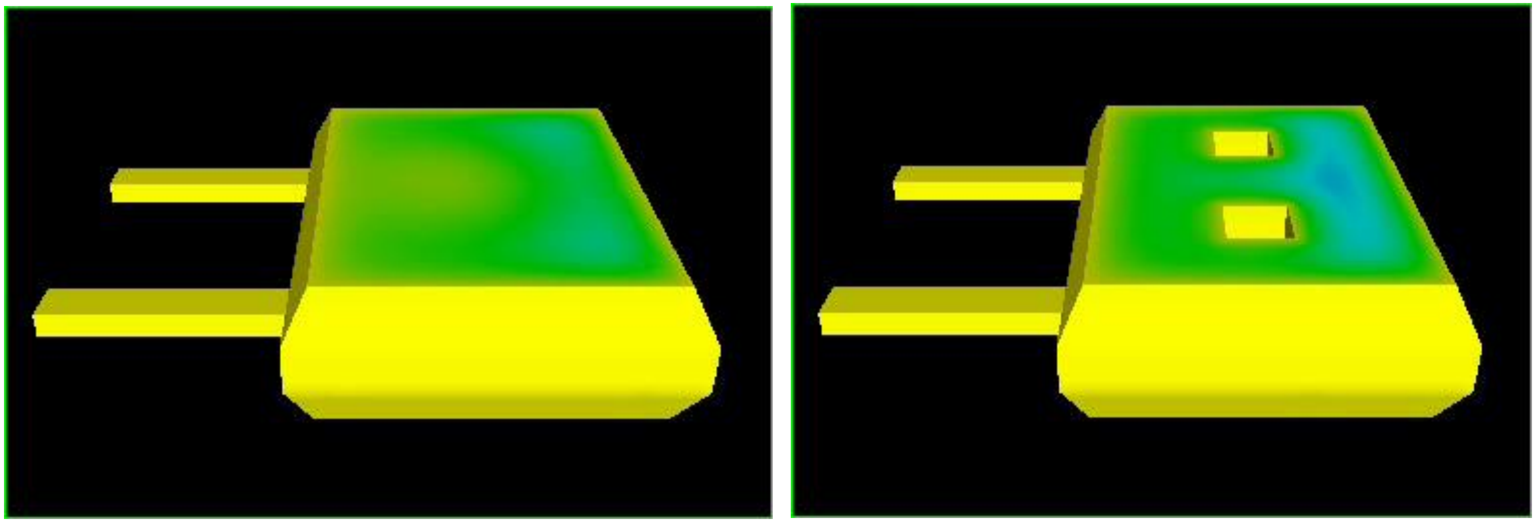
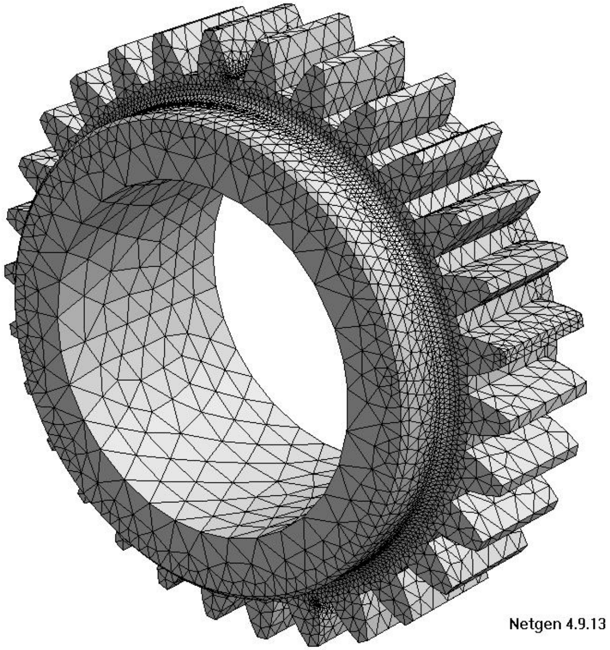


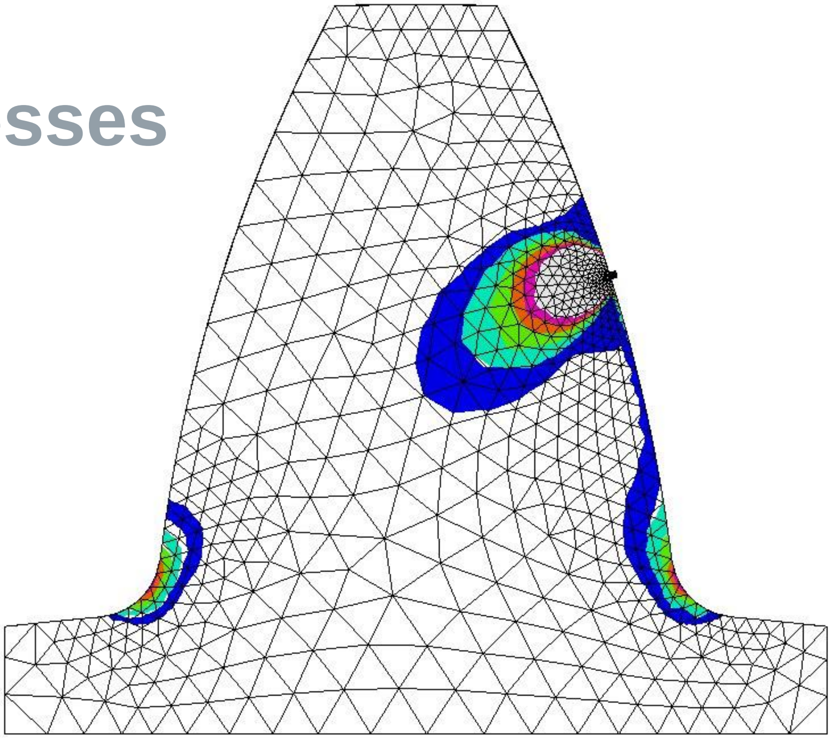
Figure by VTI Technologies

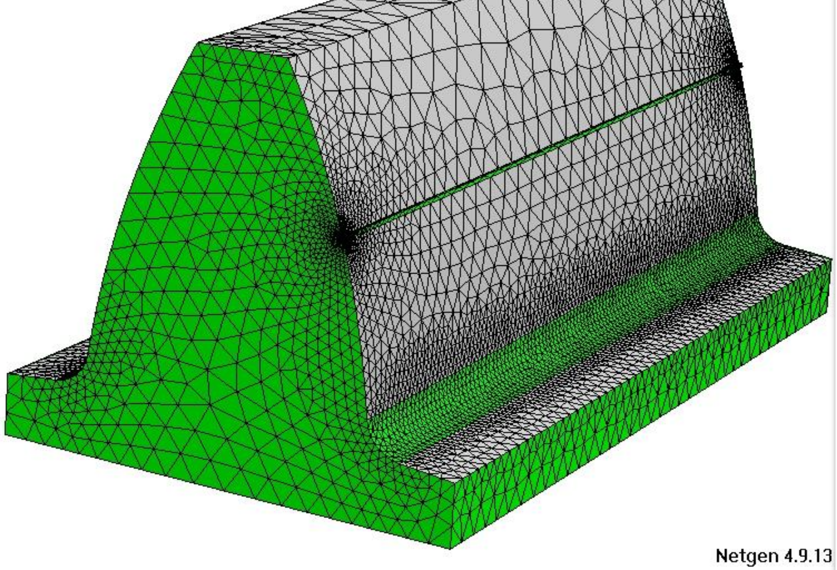


A. Pursula, P. Råback, S. Lähteenmäki and J. Lahdenperä, *Coupled FEM simulations of accelerometers including nonlinear gas damping with comparison to measurements*,
J. Micromech. Microeng. **16** (2006), 2345-2354.

# Elasticity – von Mises stresses







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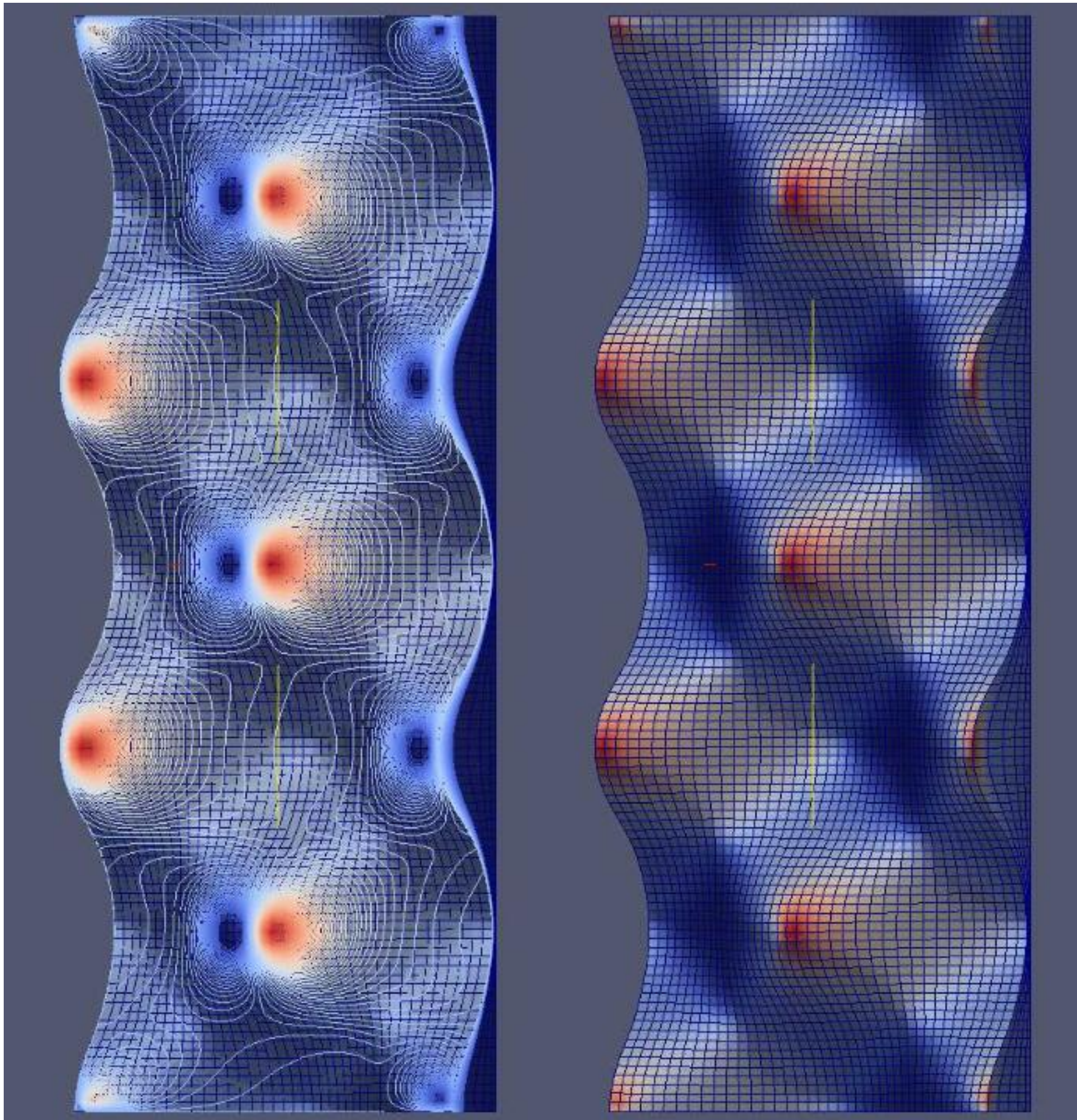
# EHDL of patterned surfaces

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

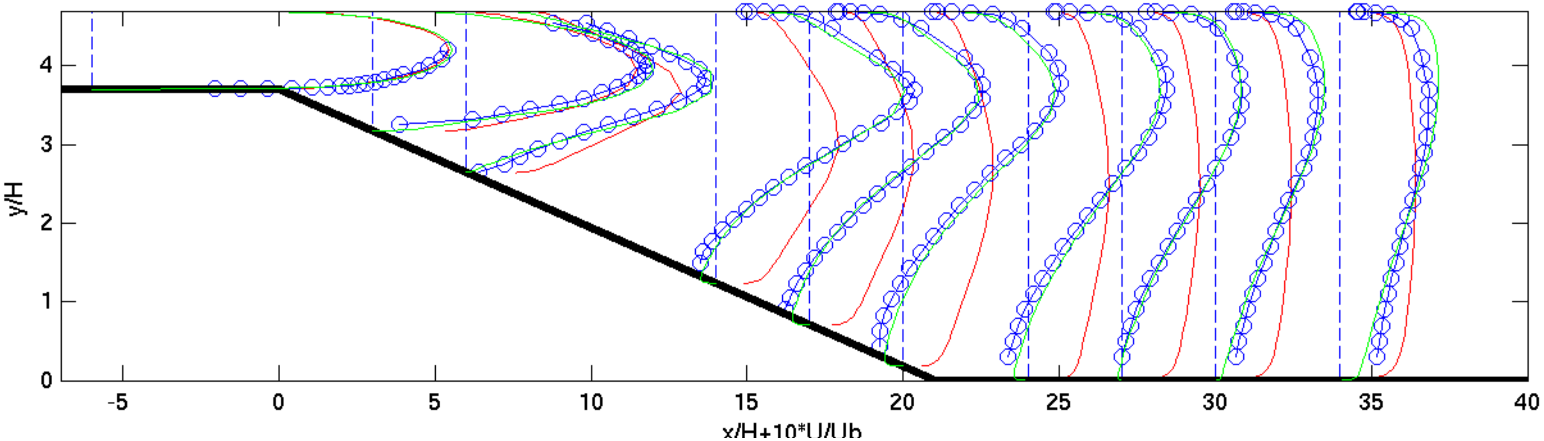


# Elmer – Fluid Mechanics

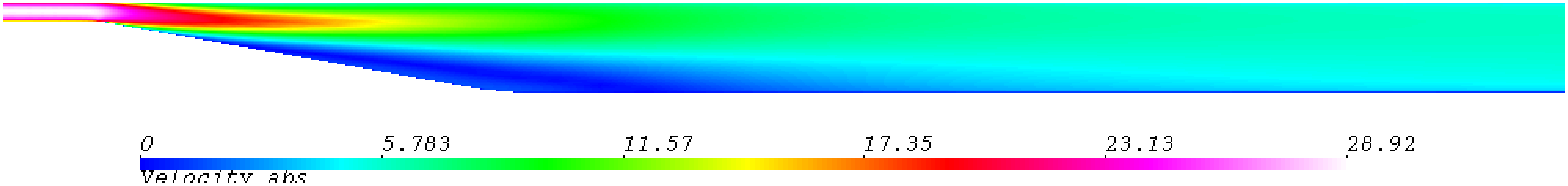
- Navier-Stokes (2D & 3D)
  - Nonnewtonian models
  - Slip coefficients
- RANS turbulence models
  - SST $k$-$\Omega$
  - $k$-$\varepsilon$
  - $v^2$-$f$
- Large eddy simulation (LES)
  - Variational multiscale method (VMS)
- Reynolds equation
  - Dimensionally reduced N-S equations for small gaps (1D & 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

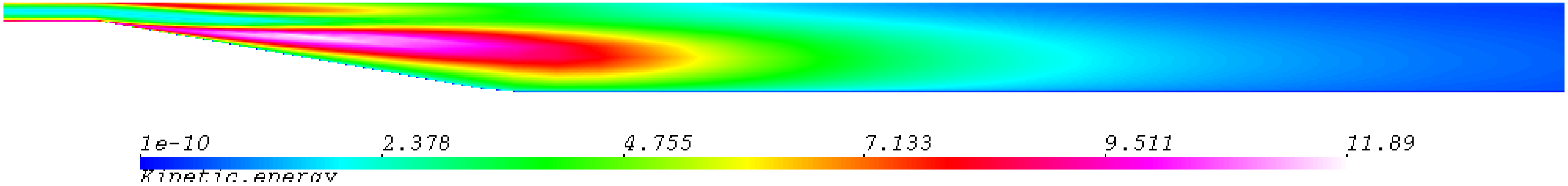
# RANS turbulence modeling

Comparison of $k$-$\varepsilon$ vs. $v^2$-$f$ –turbulence models (red



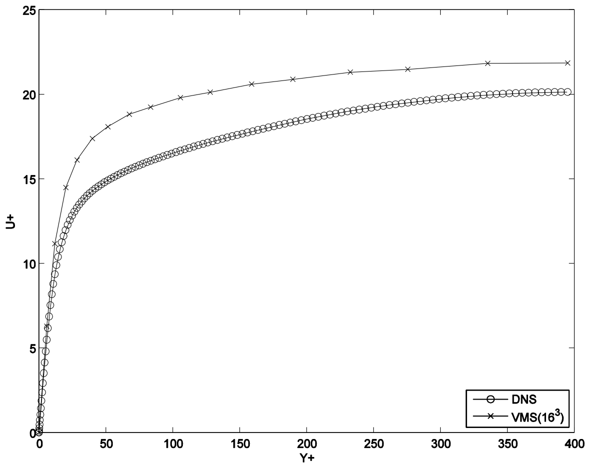
**Simulation J. Ruokolainen, CSC**



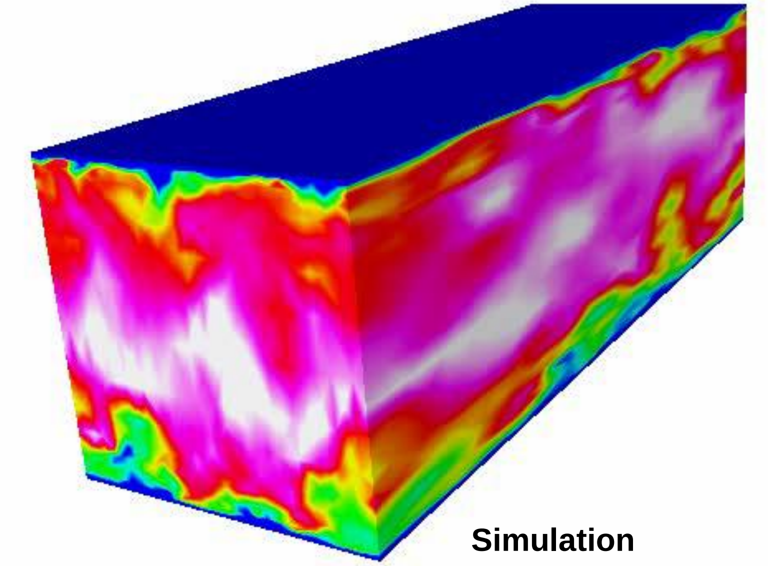


# VMS turbulence modeling

- 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



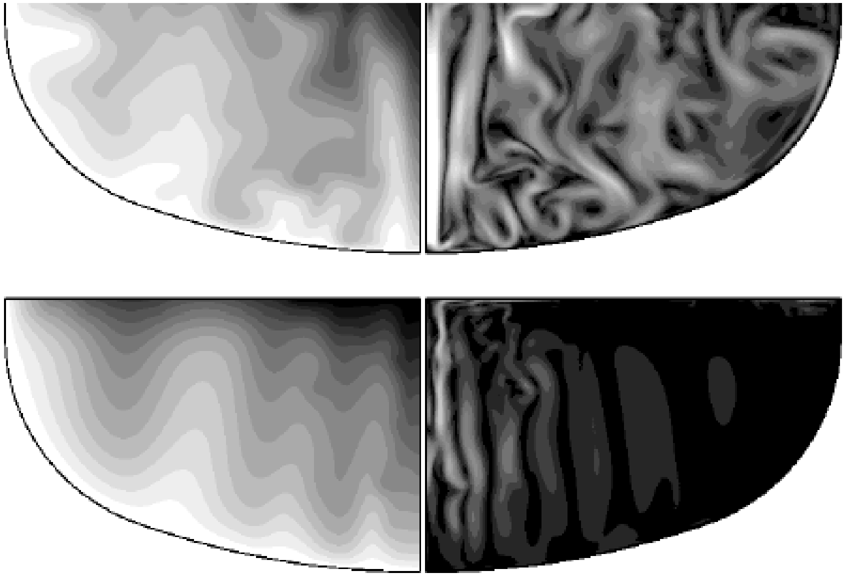
Plane flow with $Re_\tau$=395



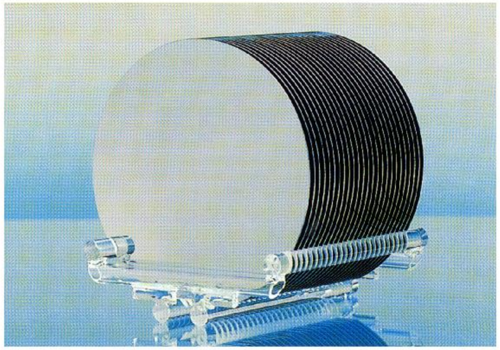
**Simulation**
**J. Ruokolainen, CSC**

# Czockralski Crystal Growth

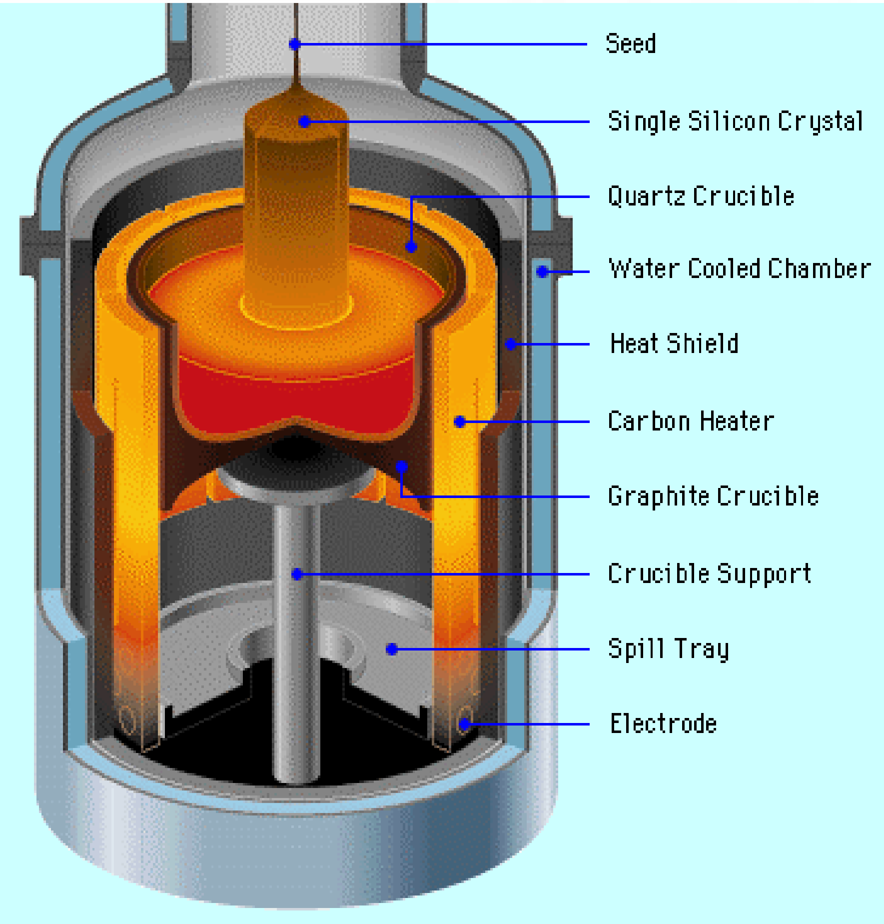
- Most crystalline silicon is grown by the Czhockralski (CZ) method
- One of the key application when Elmer development was started in 1995



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



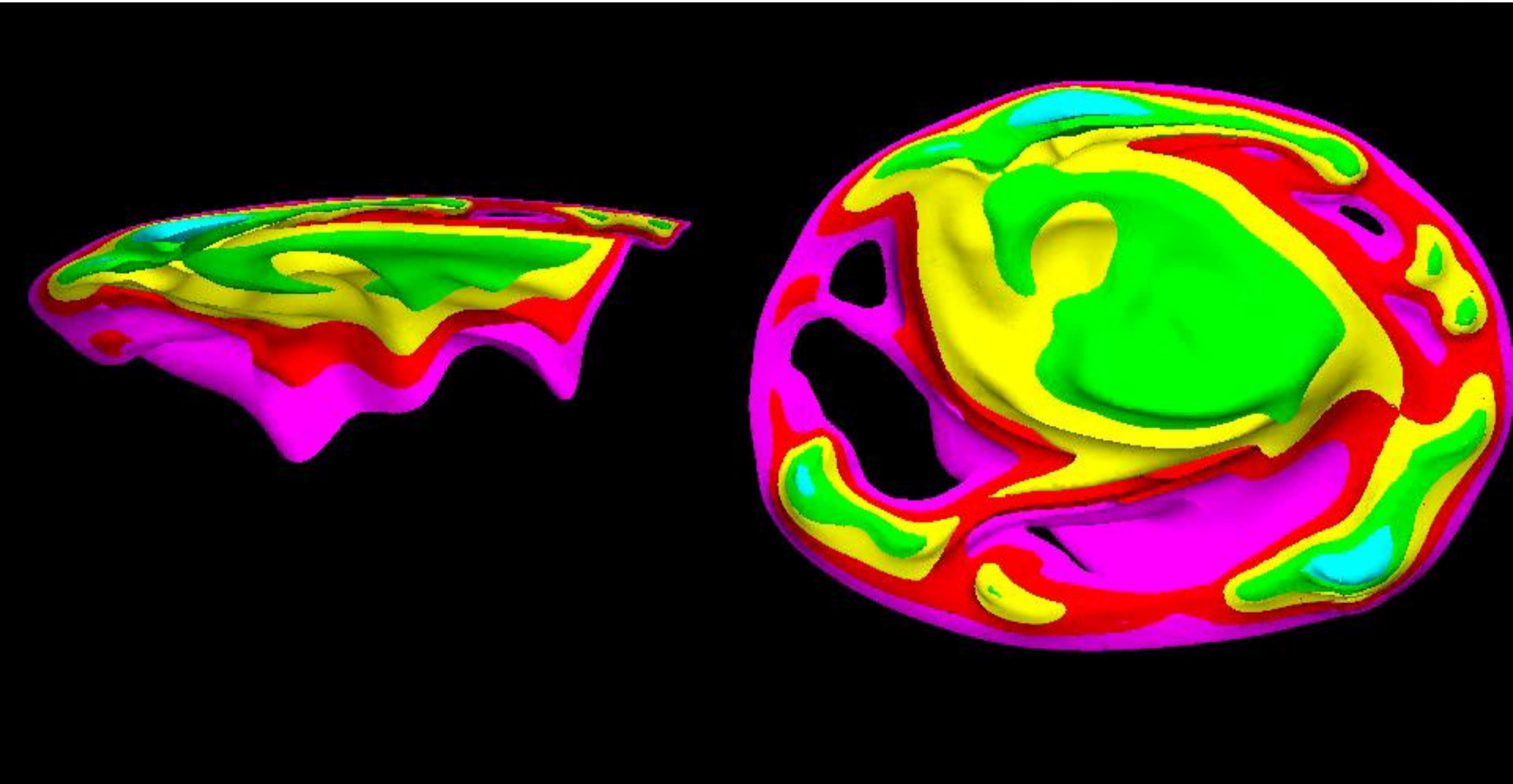
Figures by Okmetic Ltd.



# CZ-growth: Transient simulation

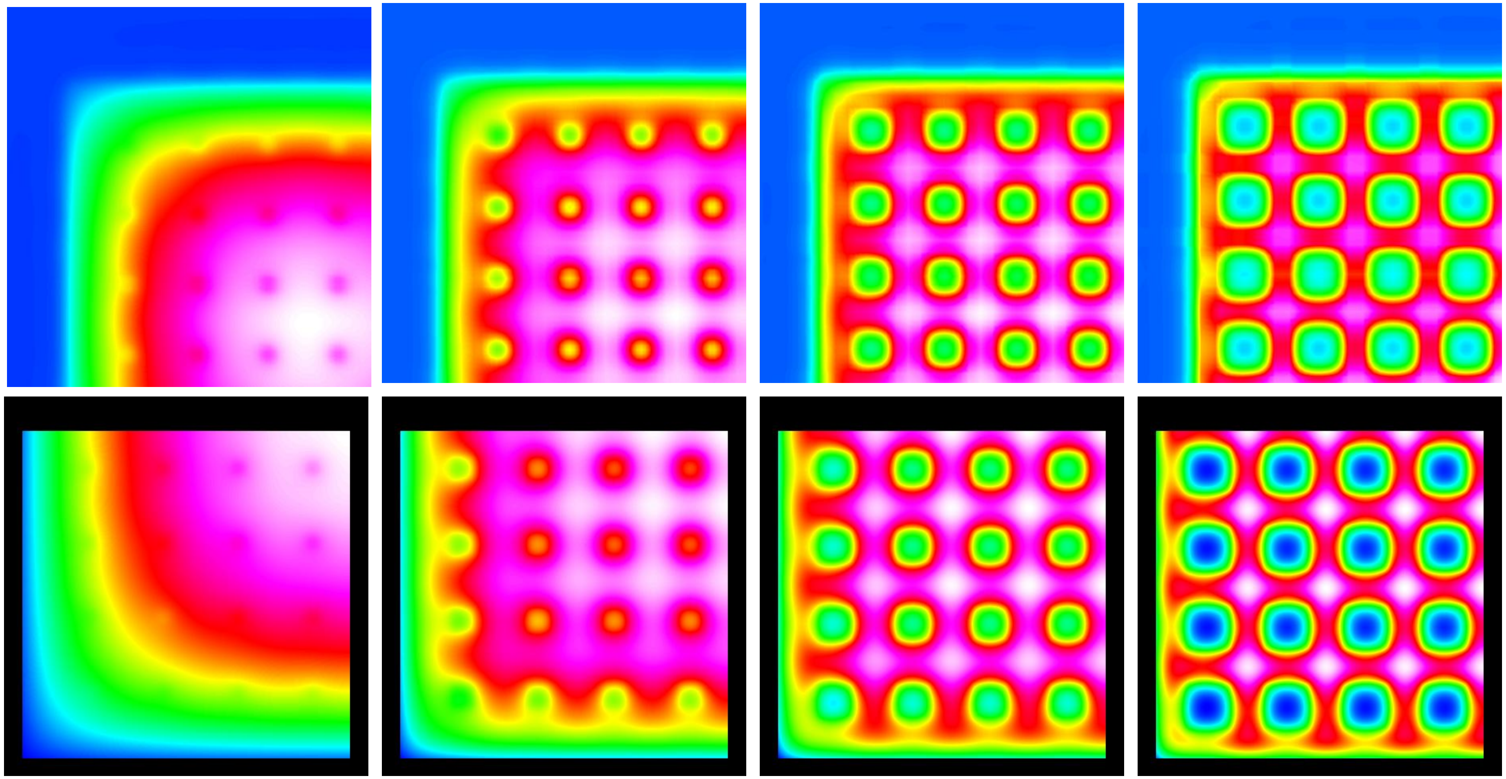
**Parallel simulation of silicon meltflows using stabilized finite element method (5.4 million elements).**

**Simulation Juha Ruokolainen, animation Matti Gröhn, CSC**



# MEMS – Perforated plates

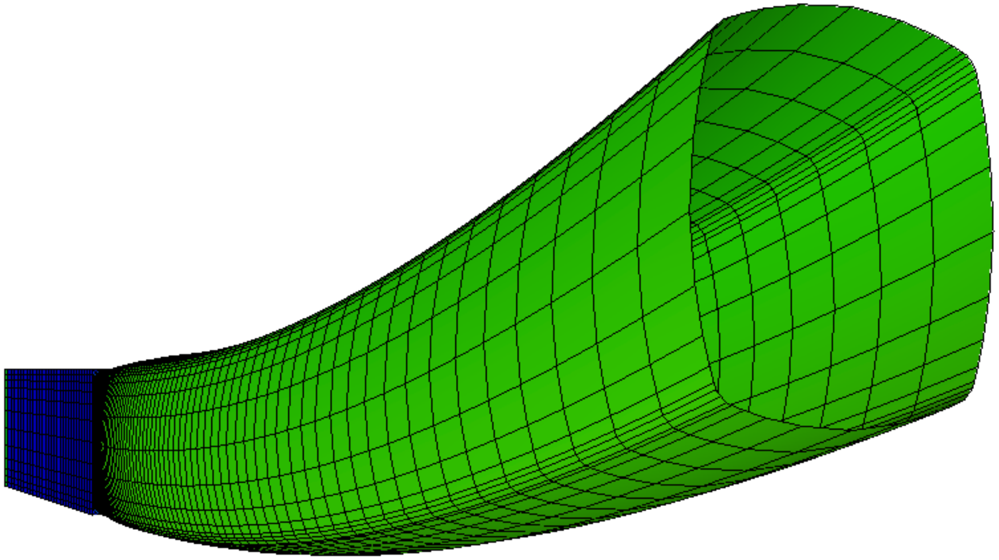
- Modified Reynolds equations may be used to model squeezed film pressure under perforated plates
- Comparison with very heavy 3D computations show good agreement (see figure)



**Simulation: Timo Veijola**

# Extrusion

- Special algorithm for the steady-state extrusion processes



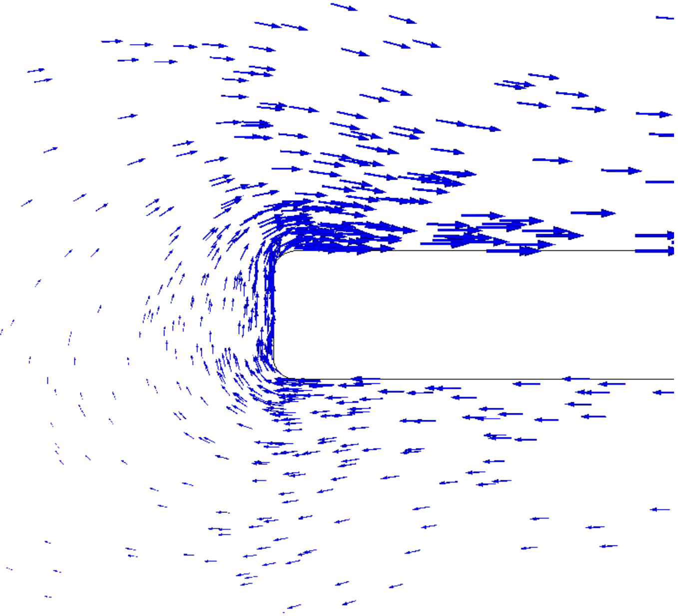
**Simulation Peter Råback, CSC**

# 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



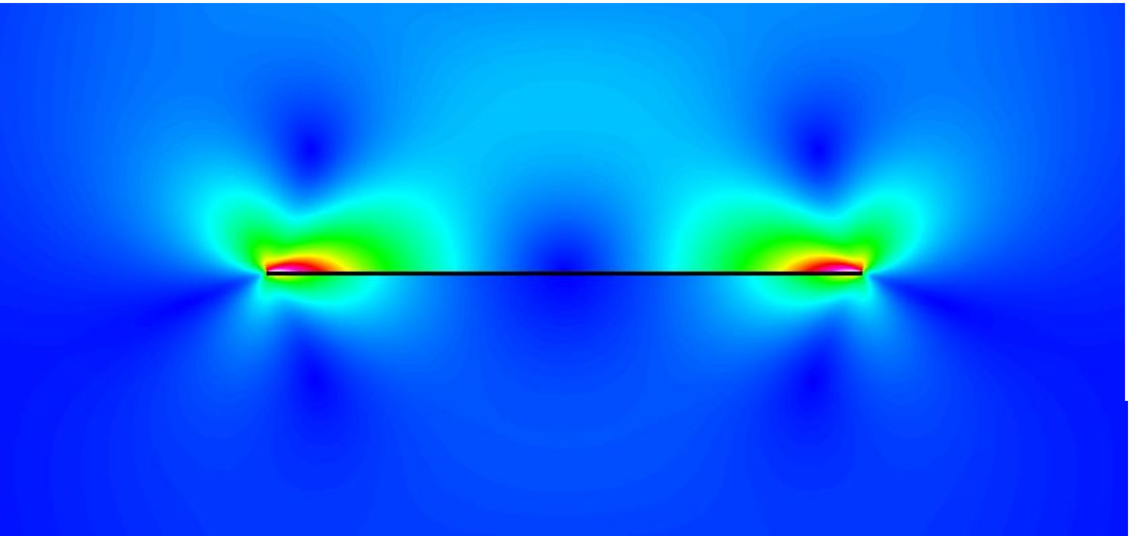
2D compressible Navier-Stokes eq. with heat eq. plus two rarefied gas effects:

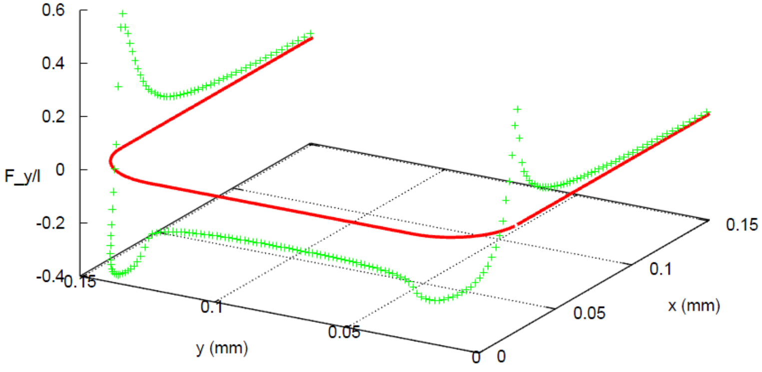
- Maxwell's wall slip and thermal transpiration

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

- Smoluchowski's temperature jump

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

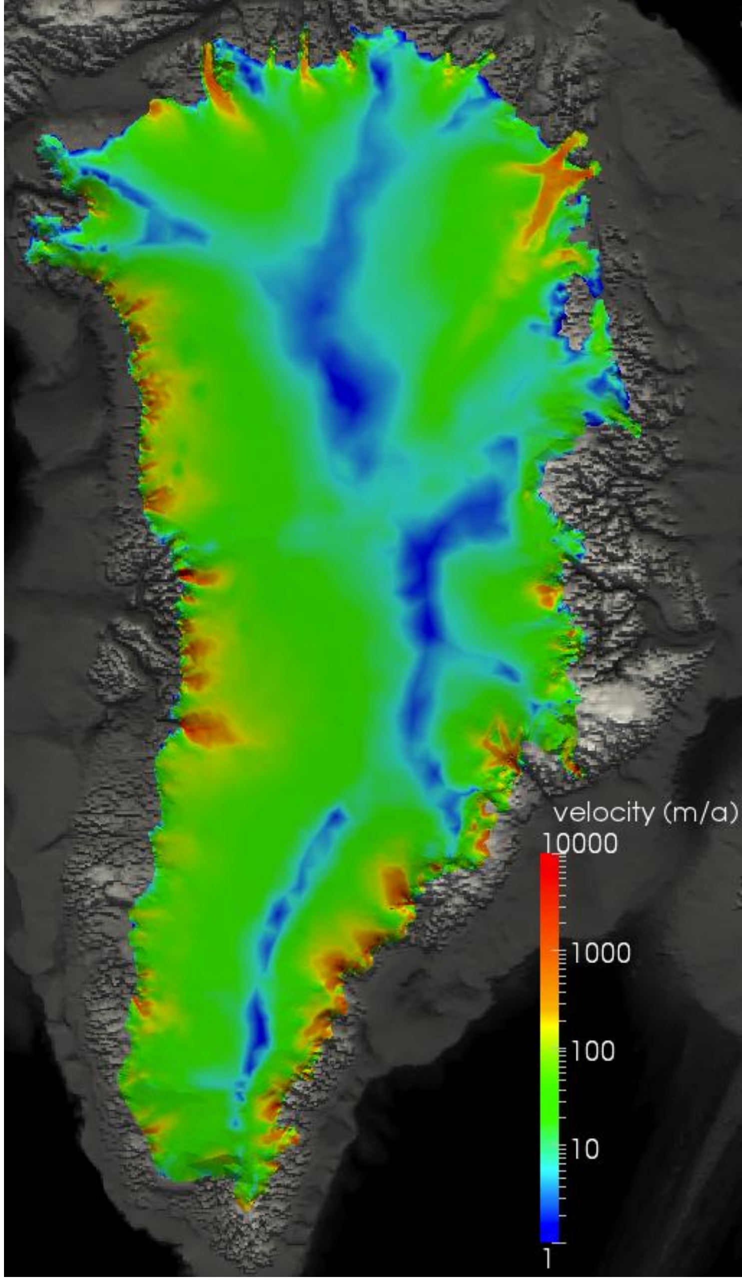




**Simulation Moritz Nadler, 2008**

# Glaciology

- Elmer is the leading code for 3D ice flow simulation
- Full Stokes equation to model the flow
- The most used full 3D Stokes tool in the area
- Continental ice sheet simulations very demanding
- Motivated by climate change and sea level rise
- http://elmerice.elmerfem.org

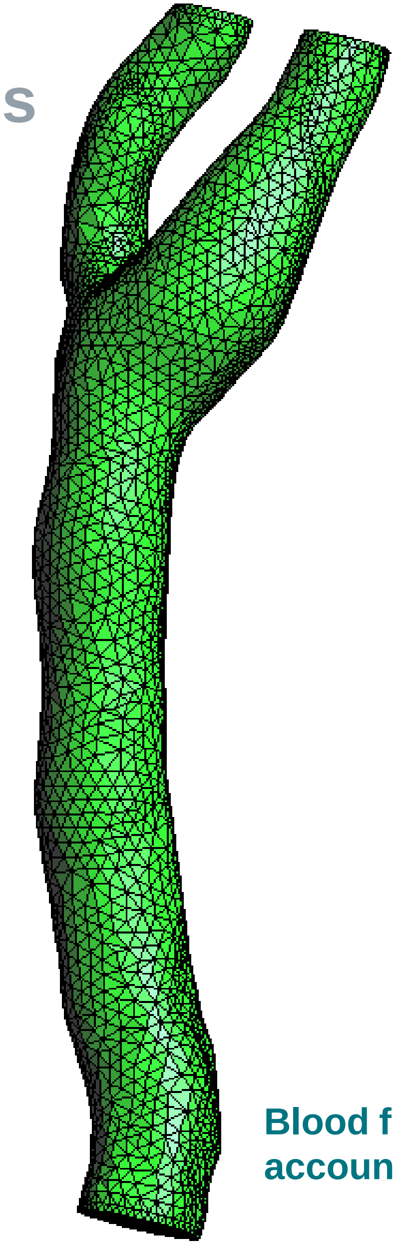


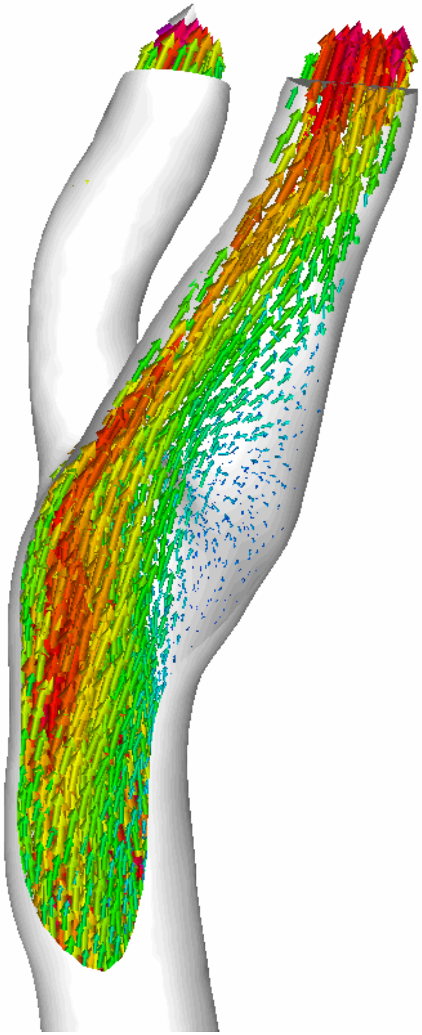
**Ice flow velocities on Greenland ice sheet. Simulation: Fabien Gillet-Chaulet, LGGE; Thomas Zwinger, CSC.**

# 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

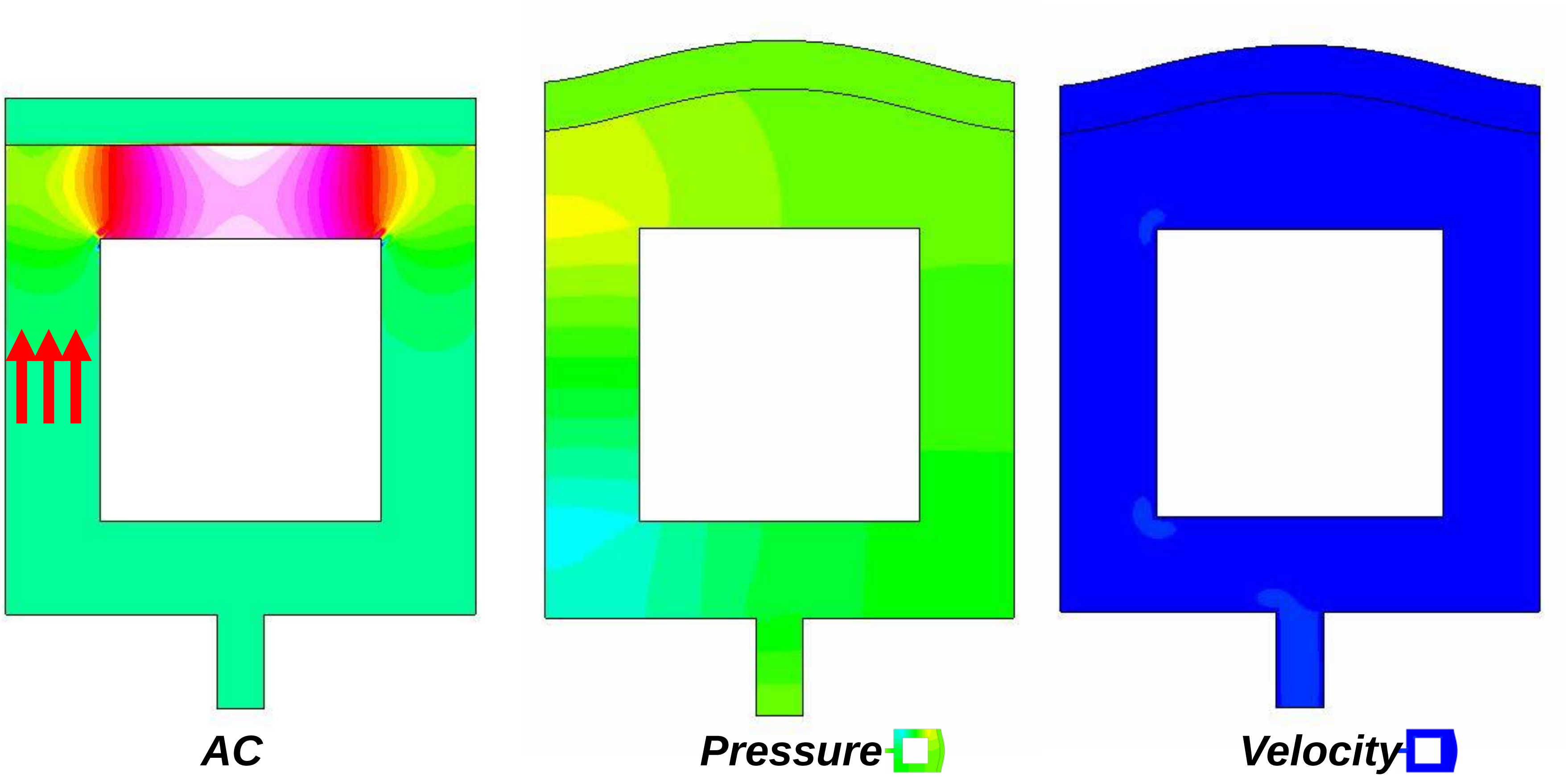




**Blood flow in carotid artery accounting FSI interaction**

# 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

# 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)
- Magnetostatics (old)
  - Axisymmetric solver for Joule heating
- MagnetoDynamics2D
  - Rotating machines
- MagnetoDynamics3D
  - AV formulation
  - 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

# Elmer and electromagnetics – historic solvers

- Electrostatics (two versions)

StatElecSolve: $-\nabla\cdot\varepsilon\nabla\phi=\rho.$

StatCurrentSolve: $\nabla\cdot\sigma\nabla\phi=\frac{\partial\rho}{\partial t}$

- StatMagSolve: (mu constant or axisymmetric)

$$\nabla\times\left(\frac{1}{\mu}\nabla\times\vec{A}\right)=\vec{\jmath}.$$

- MagenticSolve: (induction by moving charges)

$$\frac{\partial\vec{B}}{\partial t}+\frac{1}{\sigma\mu}\nabla\times\nabla\times\vec{B}-\nabla\times(\vec{v}\times\vec{B})=0,$$

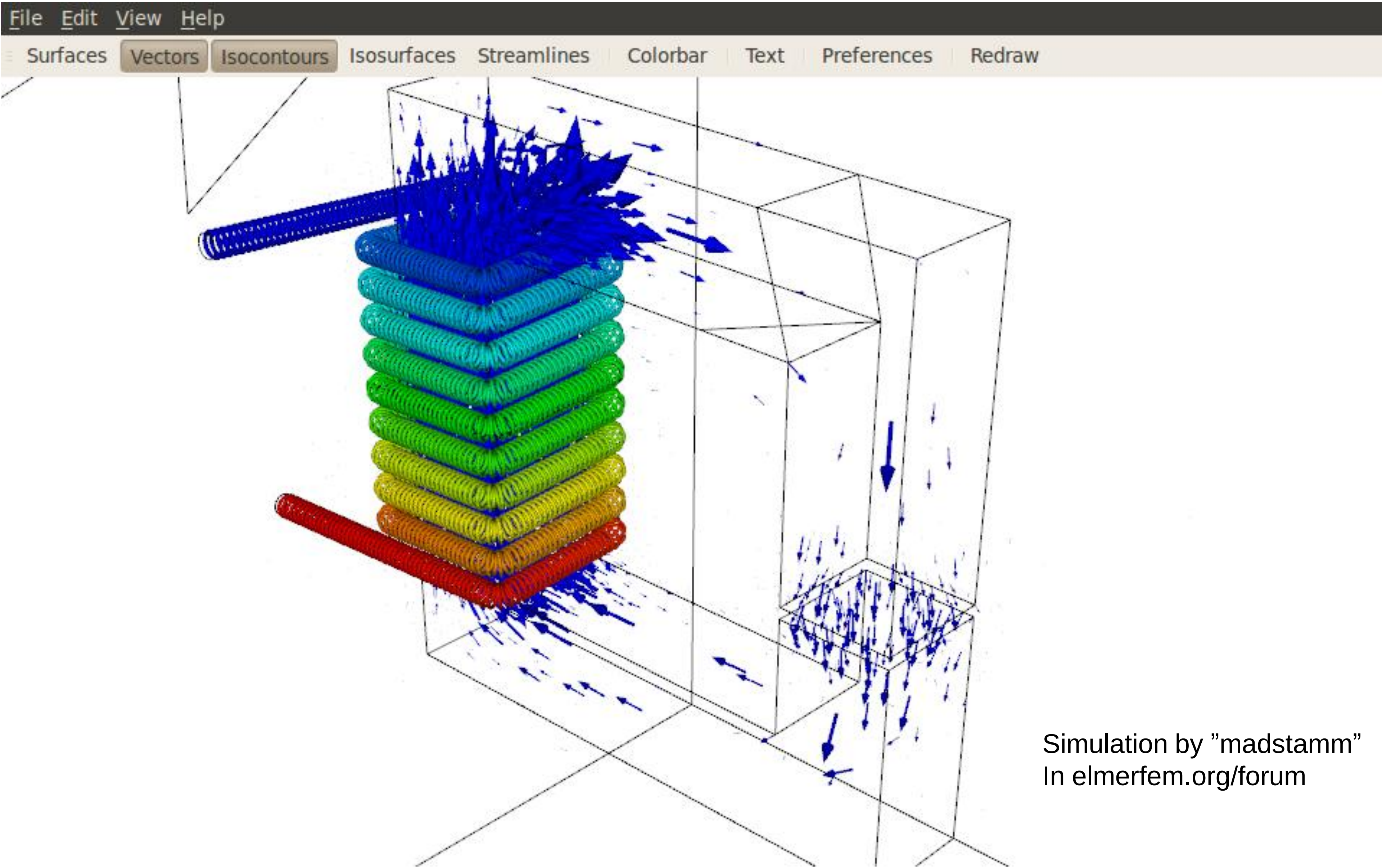
# Whitney solver for the AV formulation

- AV-formulation of the Maxwell’s equations
  - Assumes that the displacement current density is small

$$\sigma \frac{\partial \vec{A}}{\partial t} + \nabla \times \left( \frac{1}{\mu} \nabla \times \vec{A} \right) + \sigma \nabla V = \vec{J}^s + \nabla \times \vec{M}^s - \sigma \nabla V^s$$

- Coulomb gauge *div(A)=0* satisfied locally by construction by choosing Whitney elements for the basis functions for the vector potential
- Solvers also for harmonic (*d/dt* = *iω*) and steady state (*d/dt* = *0*) simulations.
- Solution of the resulting linear system may require some tailored preconditioners in large scale
- Now also a 2D version for the same equation

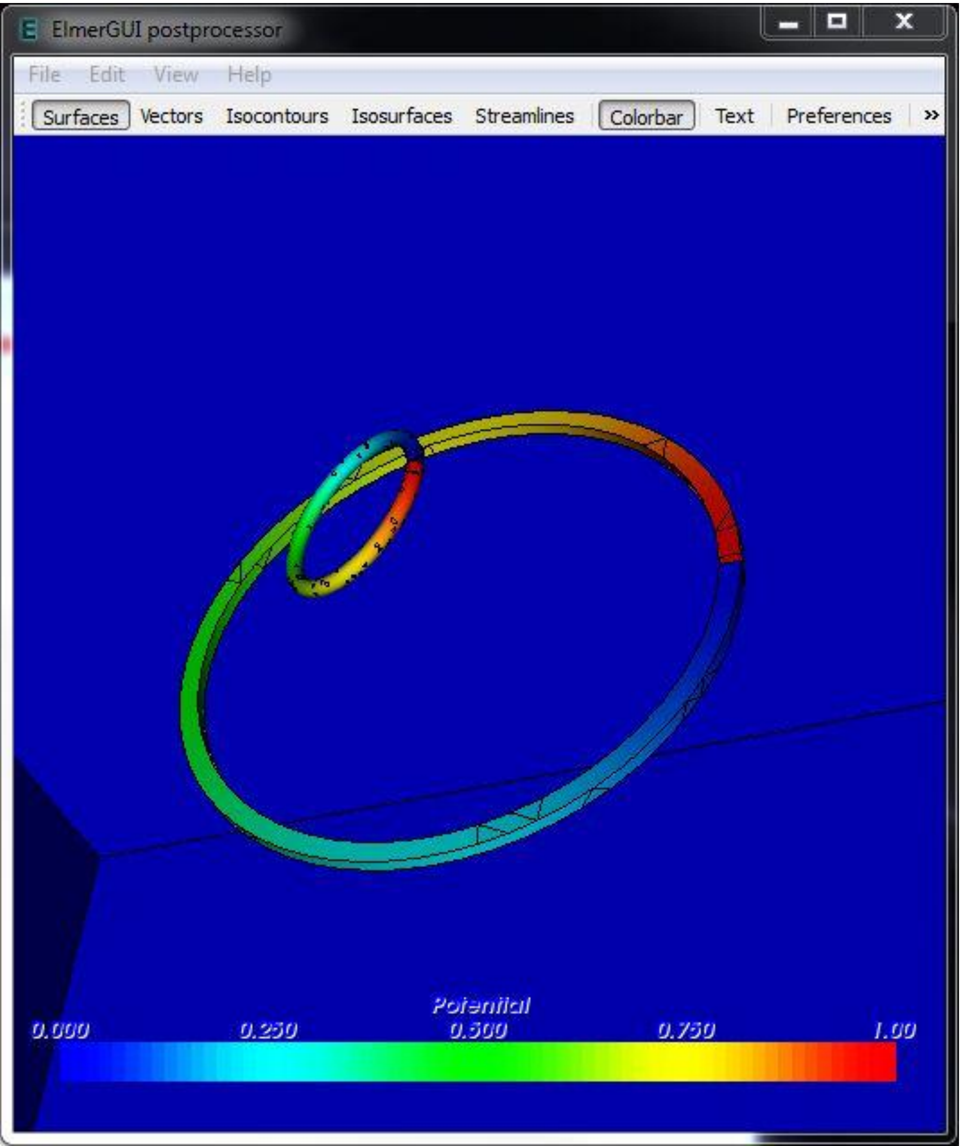
# Whitney element Solver

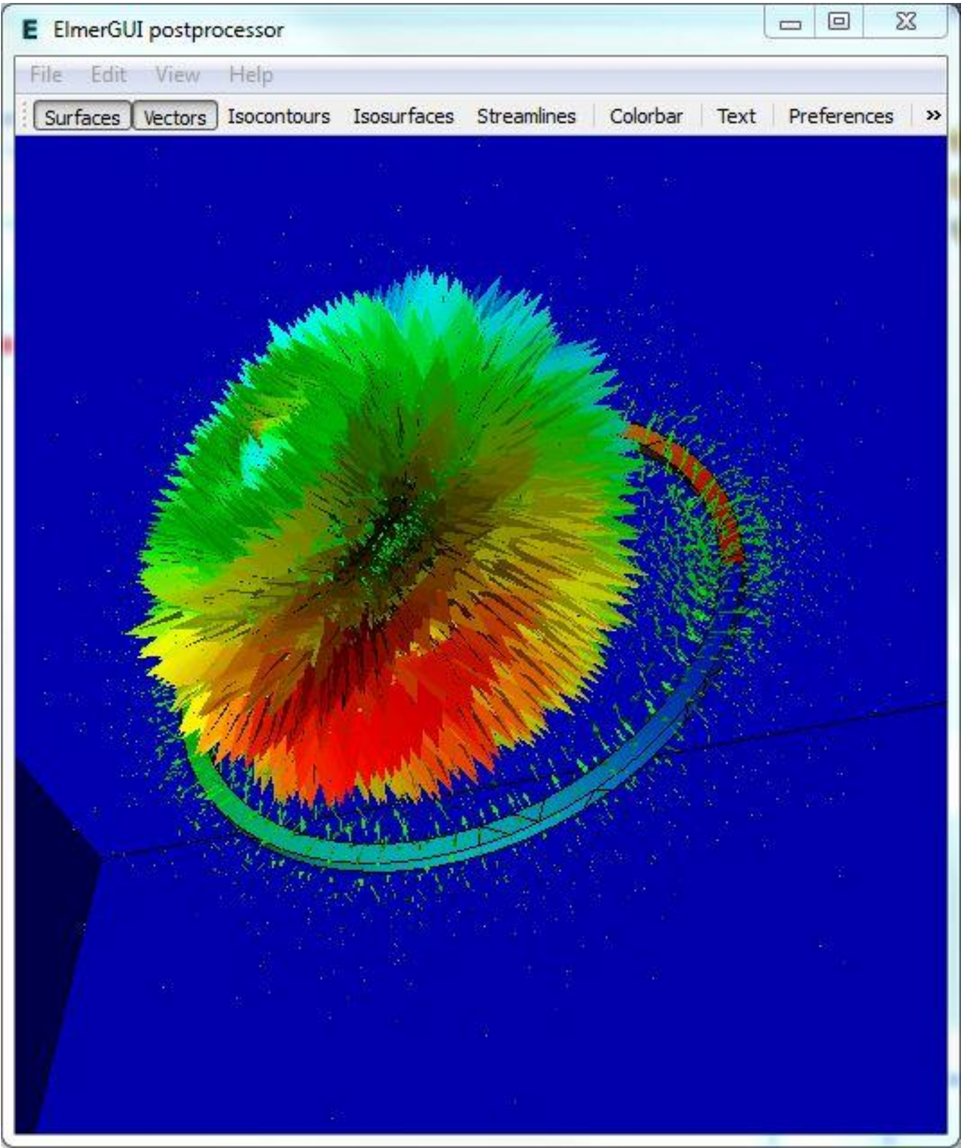


Simulation by ”madstamm”
In elmerfem.org/forum

# Mutual inductances of a coil pair

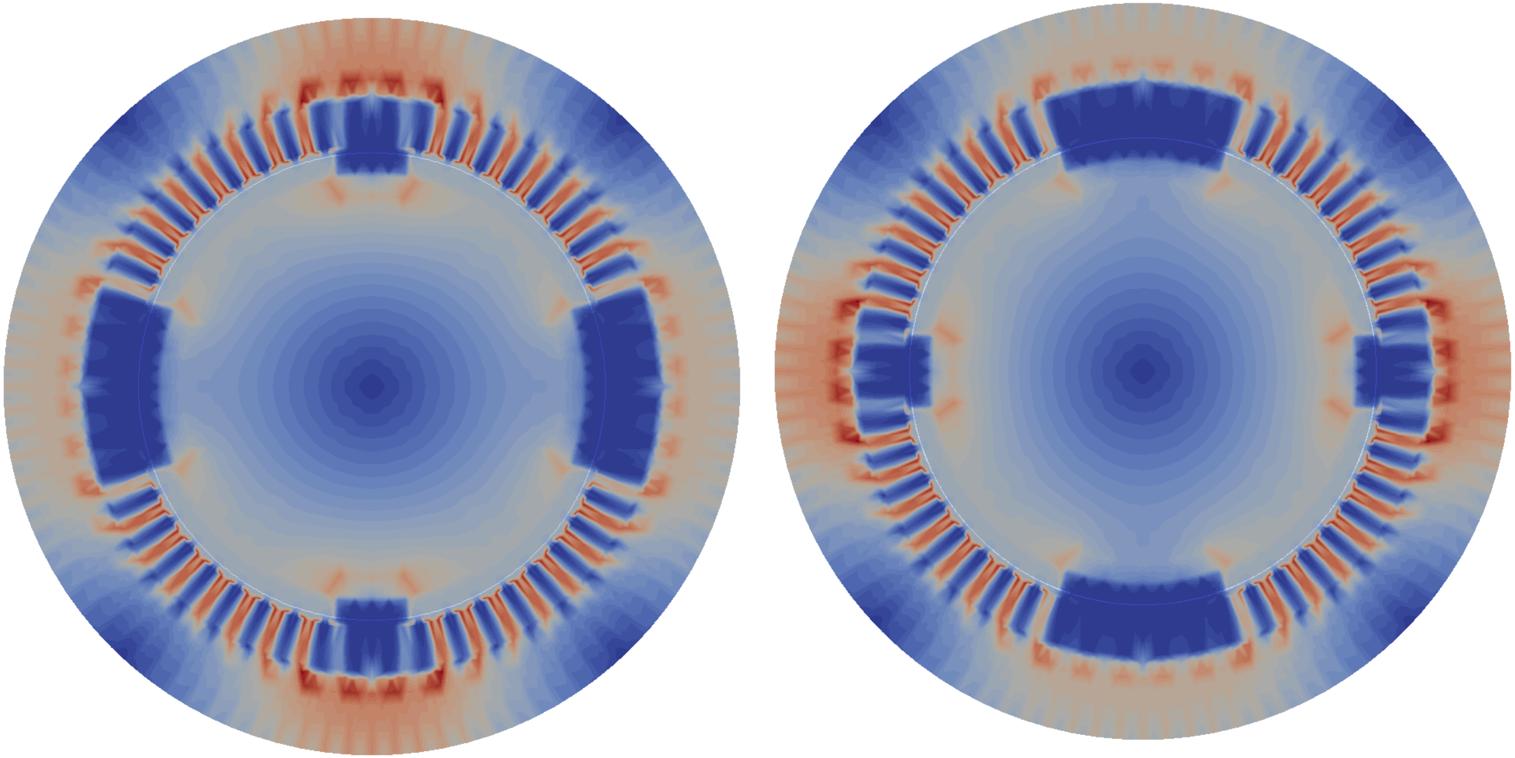
Simulation by ”millim” at elmerfem.org/forum





# Electric machine in 2D

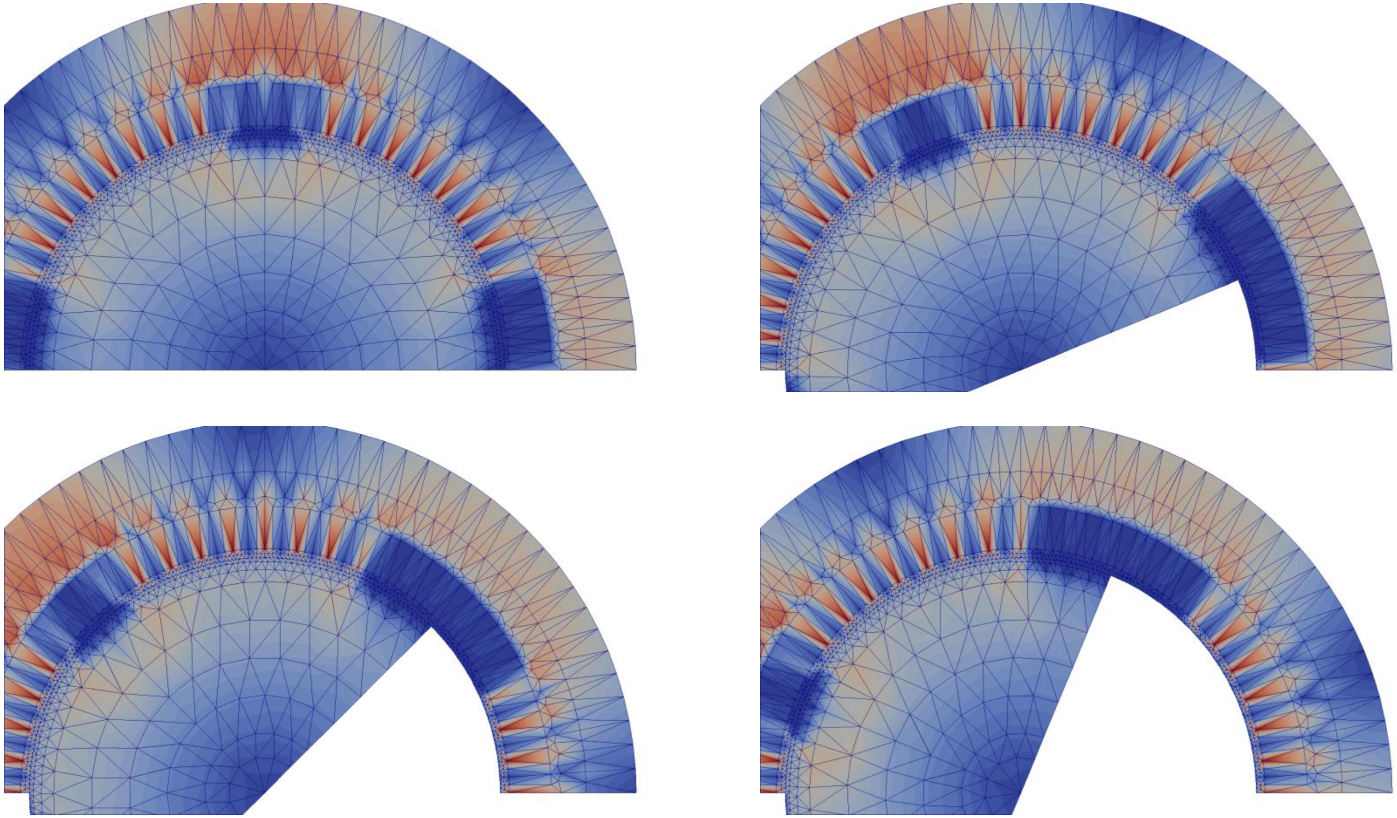
- Novel 2D vector potential solver tested with rotating BCs. Figure shows magnetic field intensity.



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

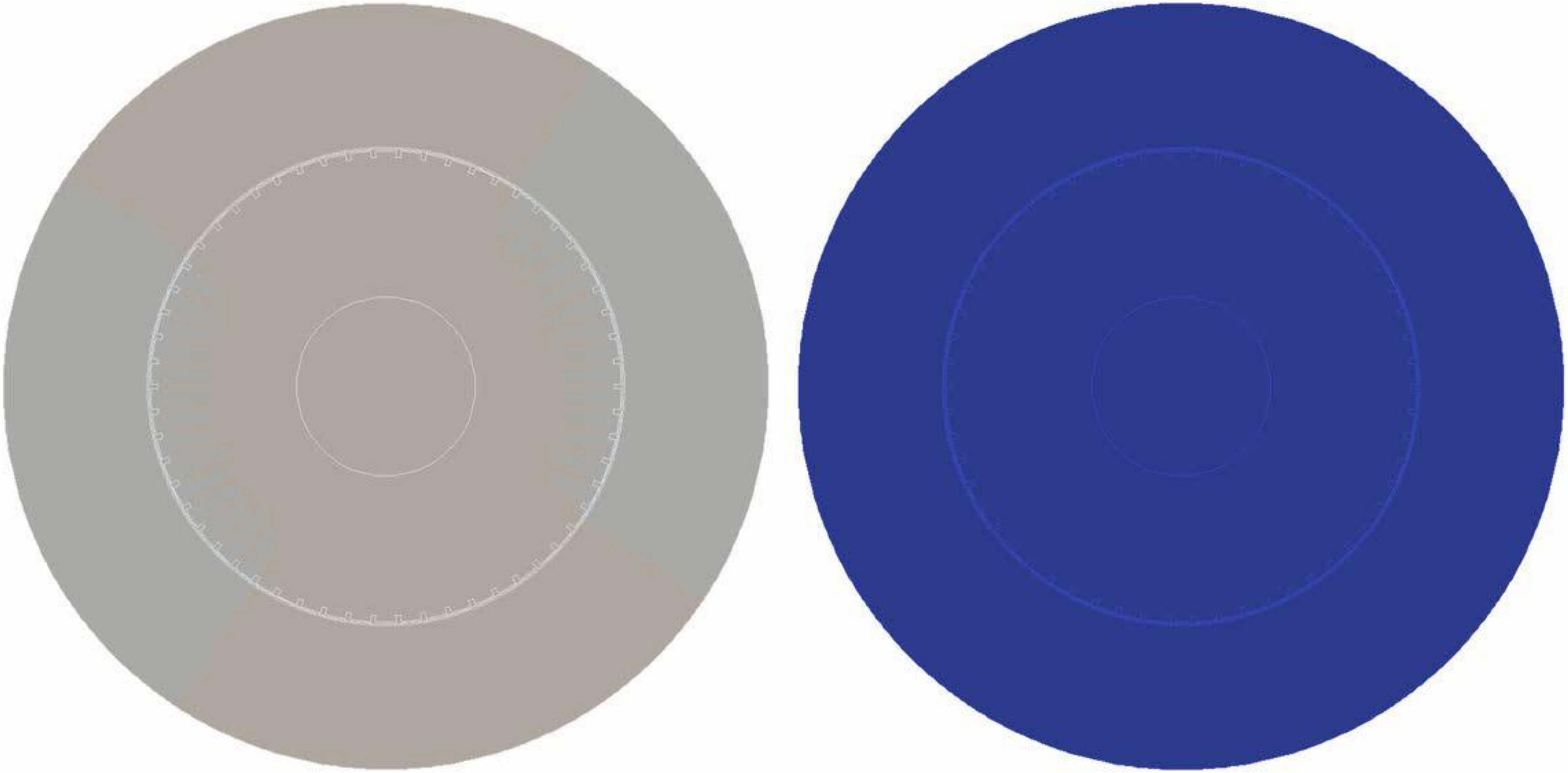
# Electric machine: Mortar finite elements

- Continuity of results between stator and rotor is ensured by mortar finite element technique
- Technique is applicable also to periodic systems



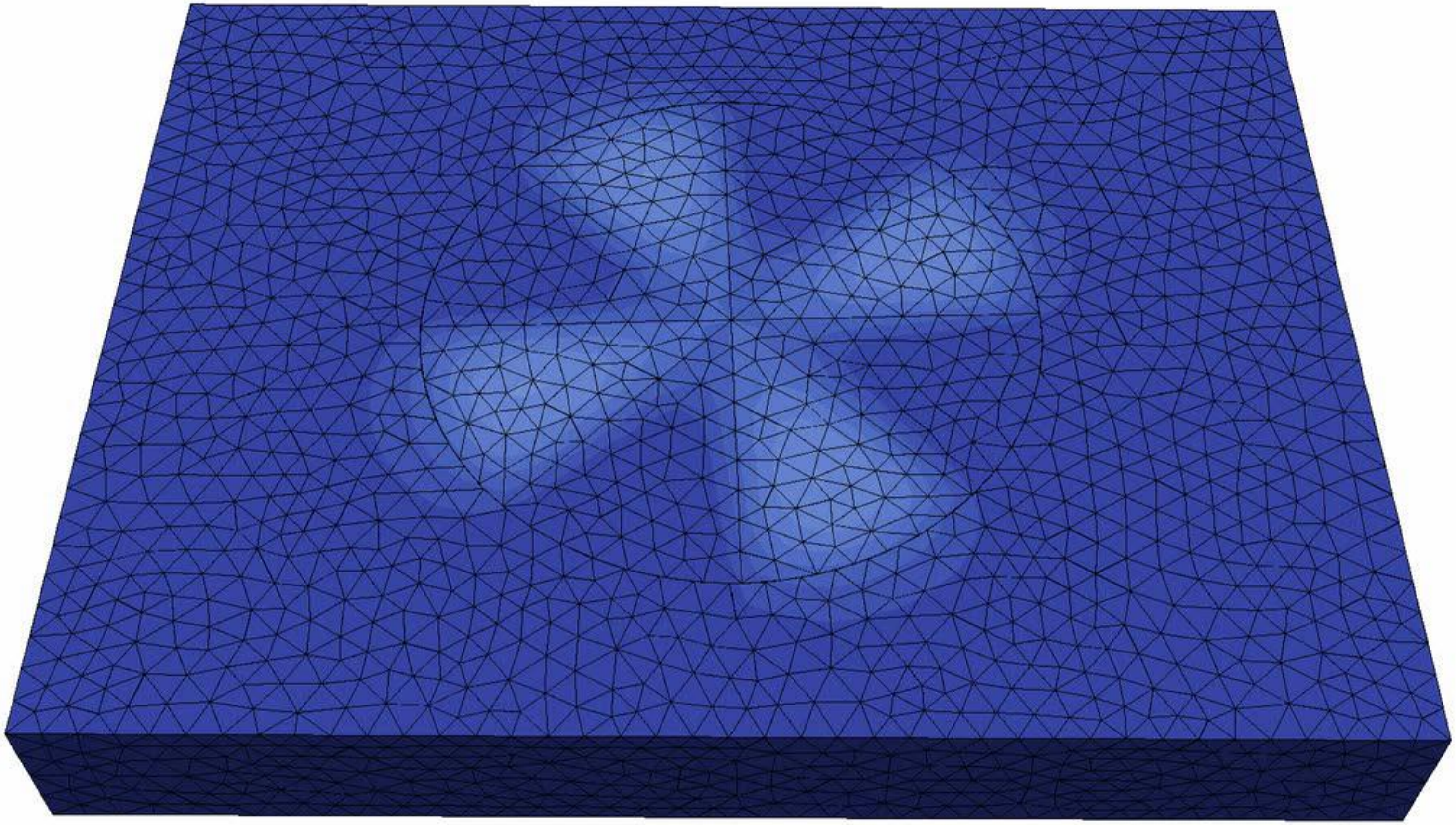
Model specification Antero Arkkio, Meshing Paavo Rasilo, Aalto Univ.
Simulation Juha Ruokolainen, CSC

# Induction machine



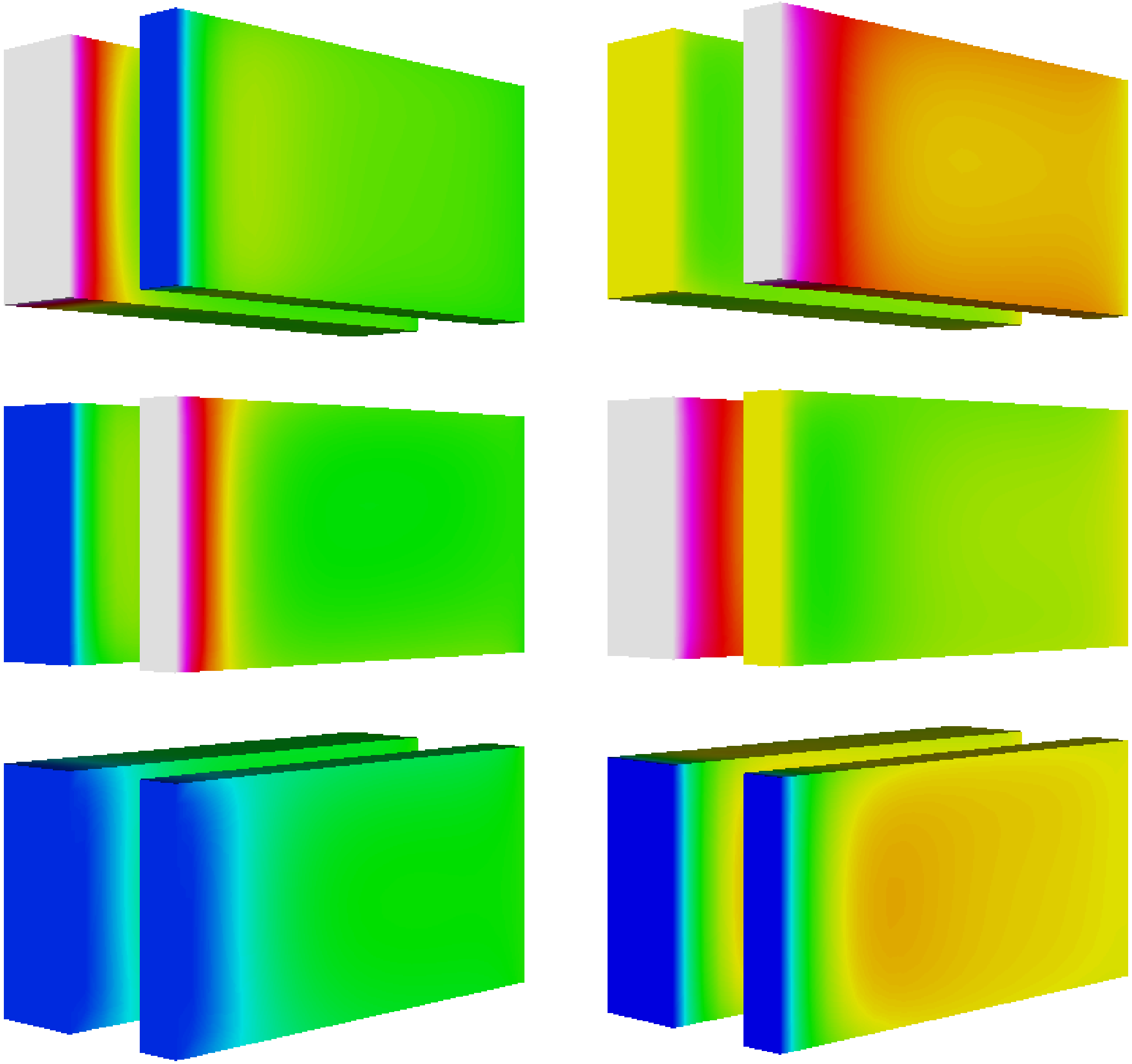
Animation: Realistic 2D induction machine depicting vector potential and magnetic field intensity. Case specification by Mikko Lyly, ABB. Model development Juha Ruokolainen, CSC. Visualization Peter Råback, CSC.

# Mortar finite elements in 3D



Animation: Continuity of solution (heat equation) is ensured in rotating nonconforming meshes. Simulation Peter Råback, CSC.

# 3-phase current – Re and Im of potential



Simulation
Peter Råback, CSC

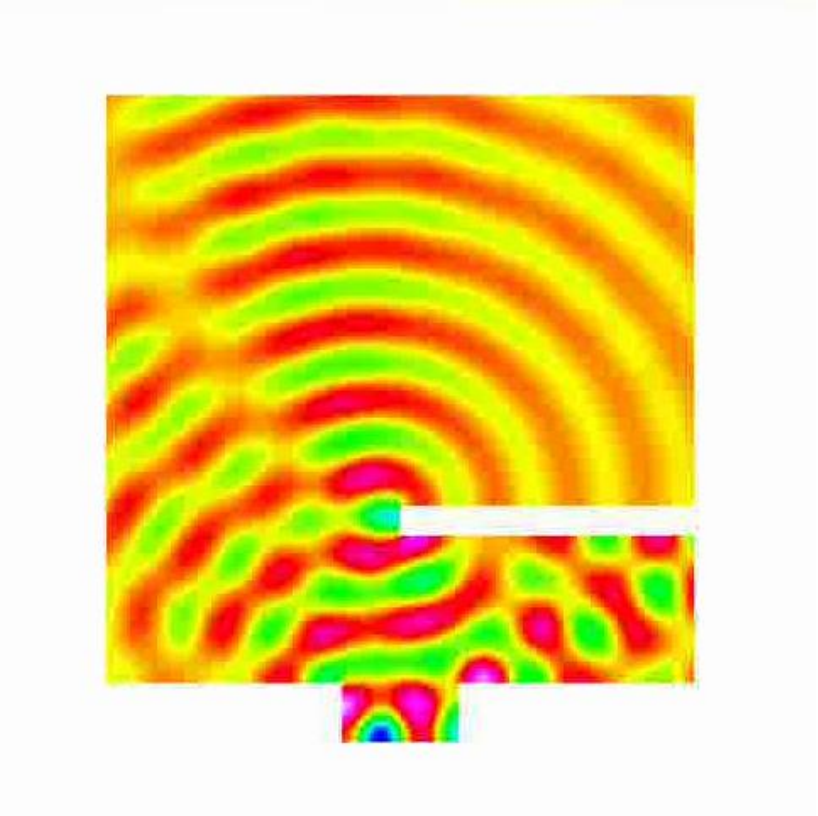
# Elmer – Acoustics

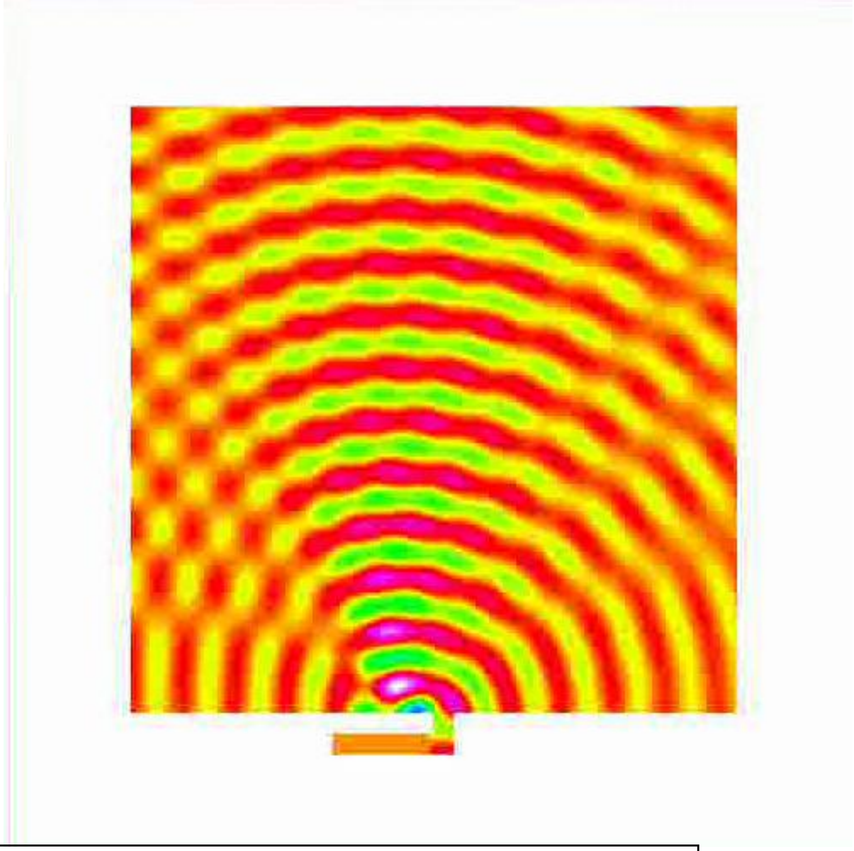
- Helmholtz Solver
  - Possibility to account for convection
- Linearized time-harmonic N-S
  - Special equation for the dissipative acoustics
- Thermal N-S
  - Ideal gas law
  - Propagation of large amplitude acoutic signals

- Associated numerical features
  - Bubble stabilization
- Typical physical couplings
  - Structural (vibroacoustics)

- Known limitations
  - Limited to small wave numbers
  - N-S equations are quite computitionally intensive

# Acoustic wave propagation



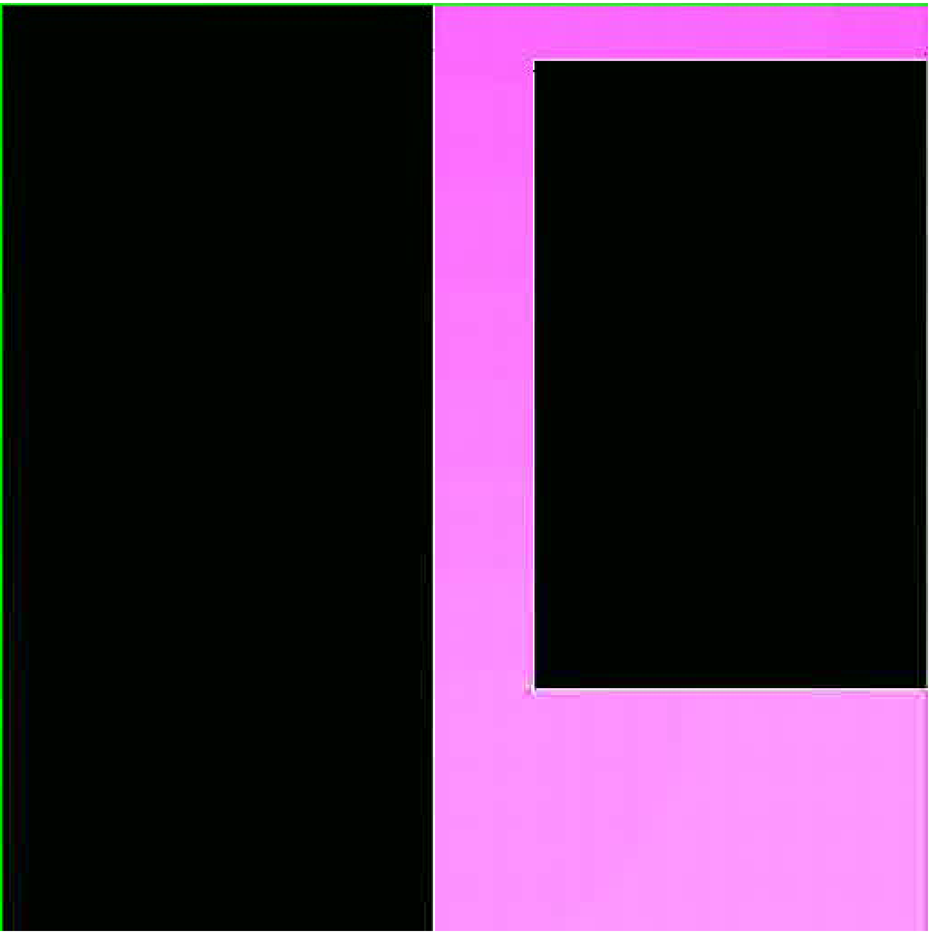


**Simulation Mikko Lyly, CSC**

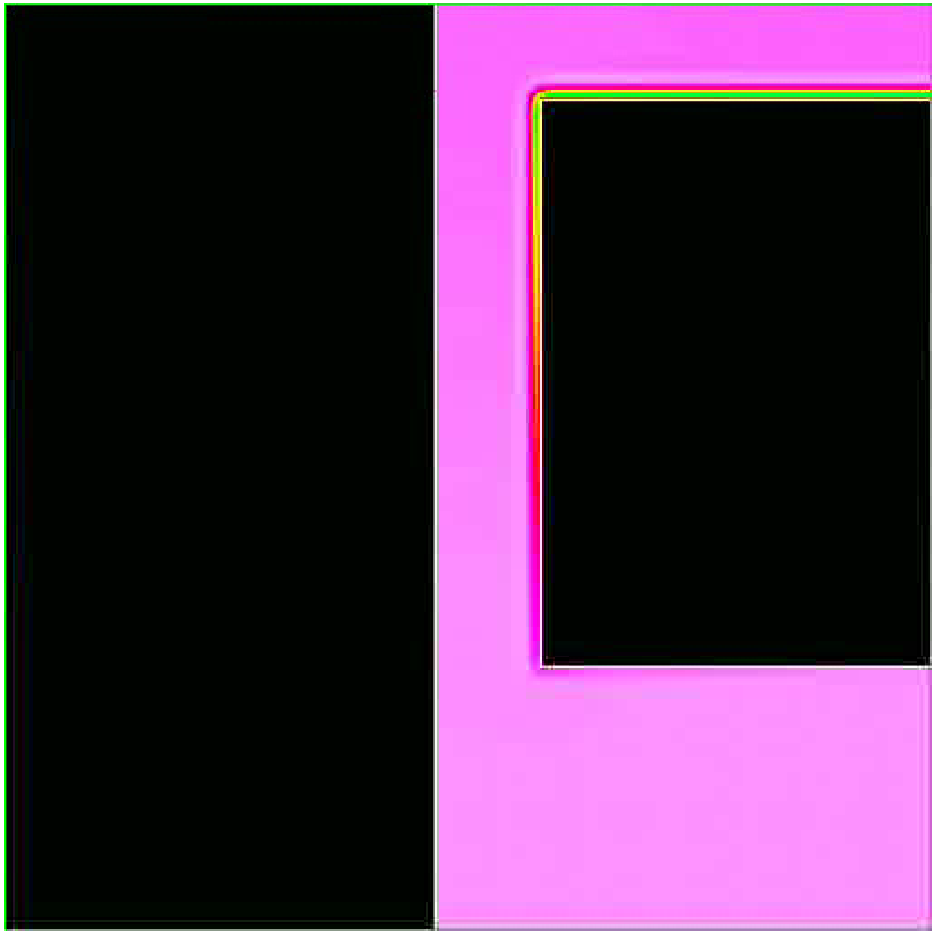
Sound waves solved from the Helmholtz equation

# Acoustics: Losses in small cavities

Temperature waves resulting from the Helmholtz equation



Temperature waves computed from the linearized Navier-Stokes equation



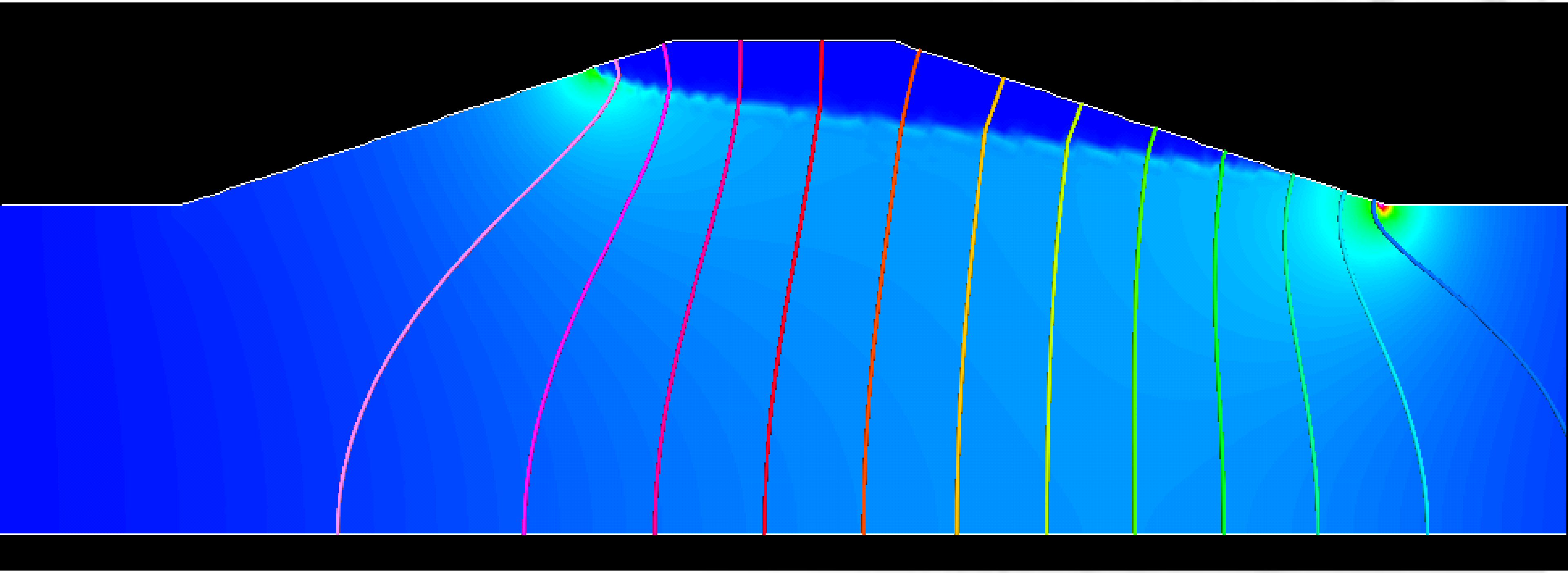
Mika Malinen, *Boundary conditions in the Schur complement preconditioning of dissipative acoustic equations*, SIAM J. Sci. Comput. 29 (2007)

# Elmer – other physical models

- Species transport
- Groundwater flow, Richards equation
- DFT, Kohn-Sham equations
- Iter reactor, fusion plasma equilibrium
- Optimization
- Particle tracking
- …

# 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

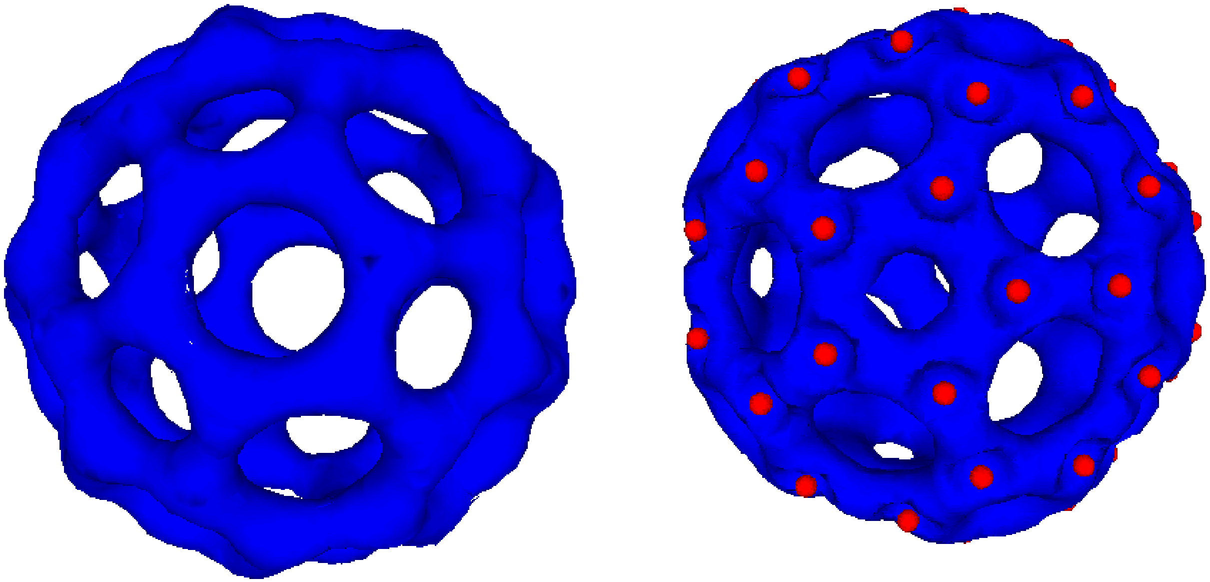


Simulation, Peter Råback, CSC

# Quantum Mechanics

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

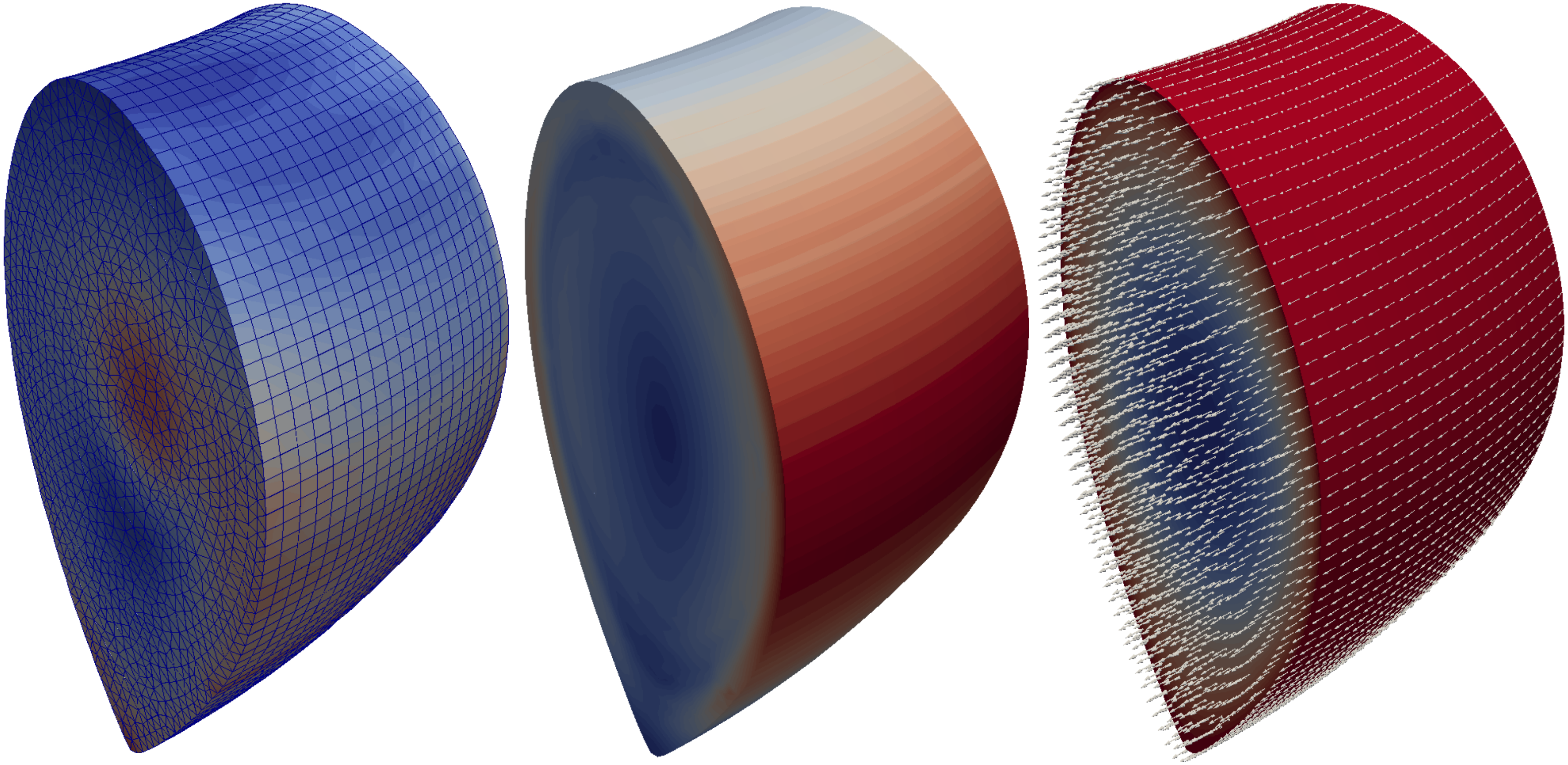
- Charge density and wave function of the 61st eigenmode of fullerine C60
- All electron computations using 300 000 quadratic tets and 400 000 dofs



Simulation Mikko Lyly, CSC

# Iter fusion reactor

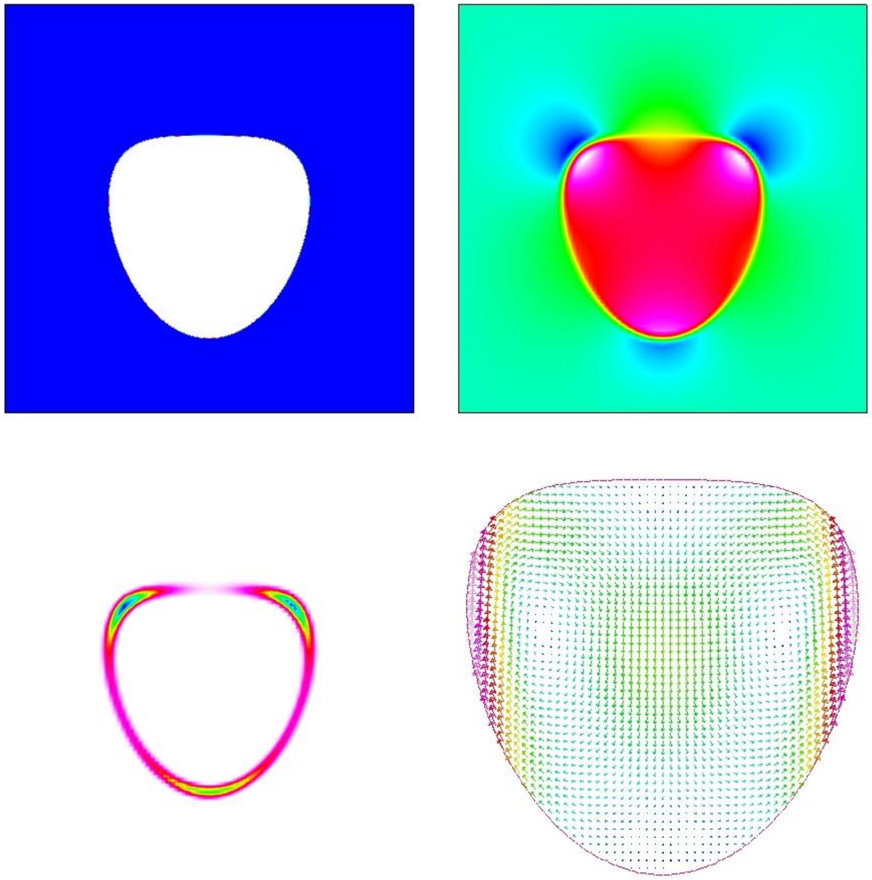
- Assumption that 2D dependencies are valid also on a perturbed 3D system
- 3D magnetic fields but no real plasma simulation

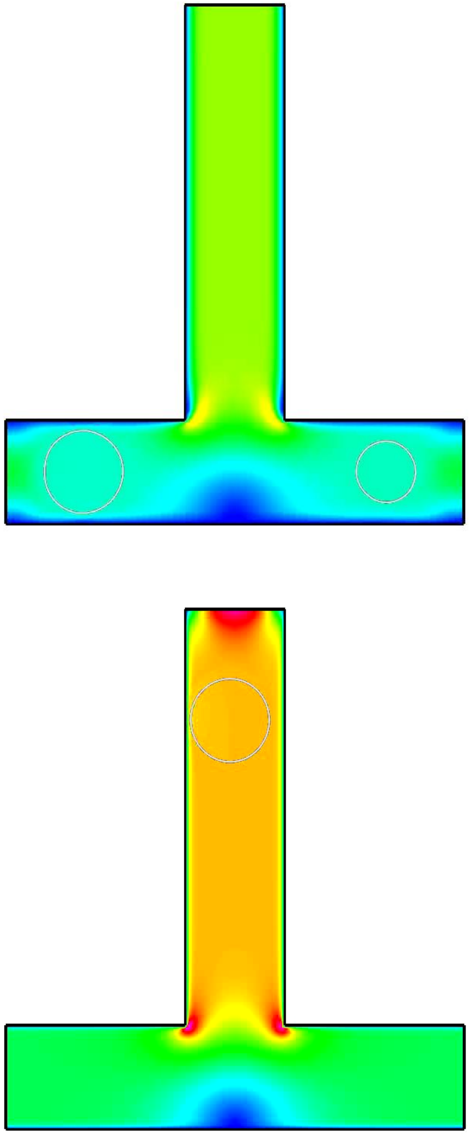


Simulation Peter Råback, CSC, 2013

# Levelset method

- 2D levelset of a falling bubble

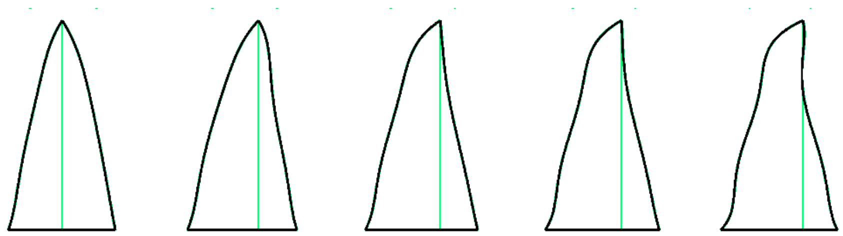




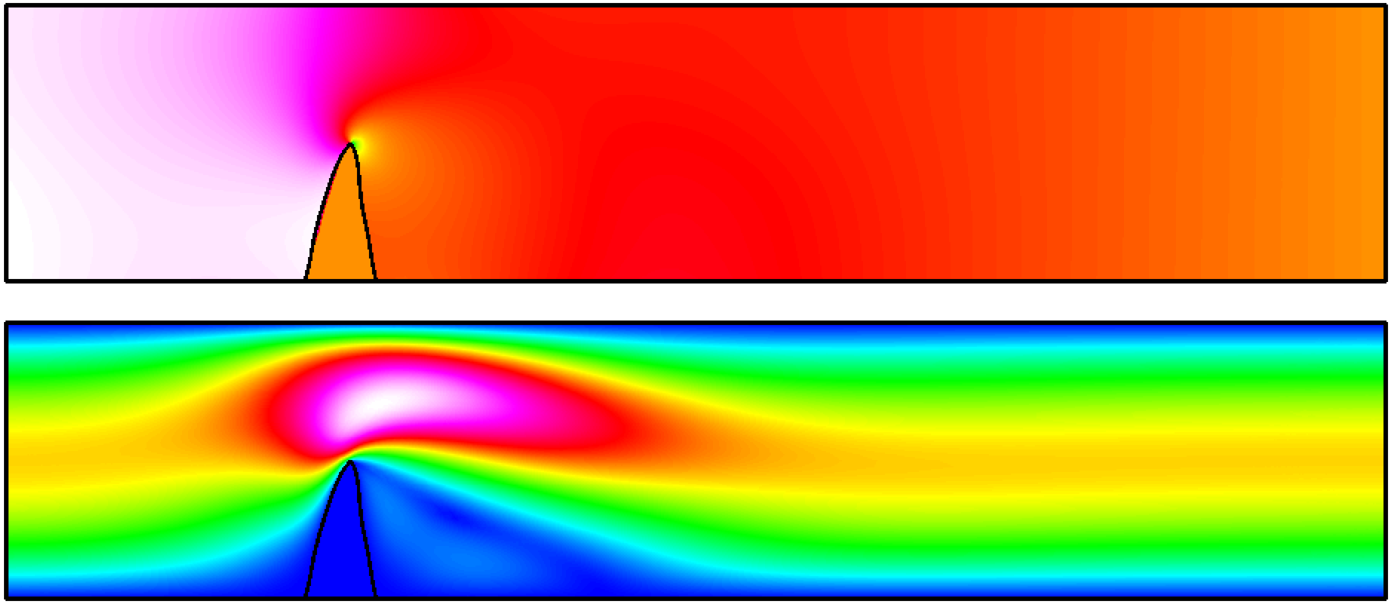
**Simulation Peter Råback, CSC**

# 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



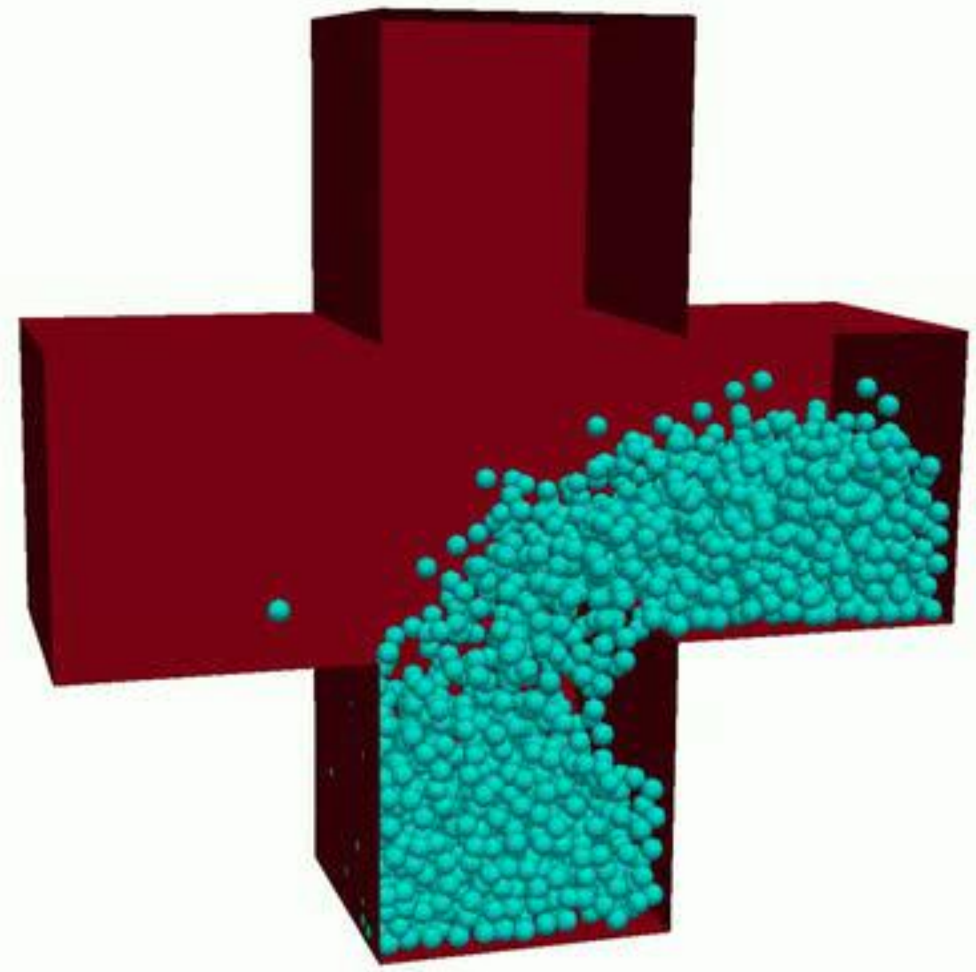
**Optimized profiles for Re={0,10,50,100,200}**



**Pressure and velocity distribution with Re=10**

**Simulation Peter Råback, CSC**

# Particle tracker - Granular flow



Simulation Peter Råback, CSC