

Elmer – an Open Source Finite Element Software for Multiphysical Problems

Thomas Zwinger

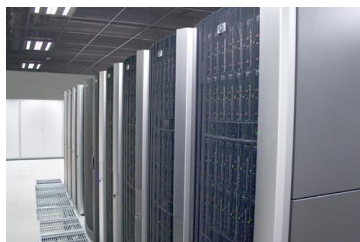
Based on slides from Peter Råback
CSC, Finnish IT Center for Science

Elmer/Ice workshop

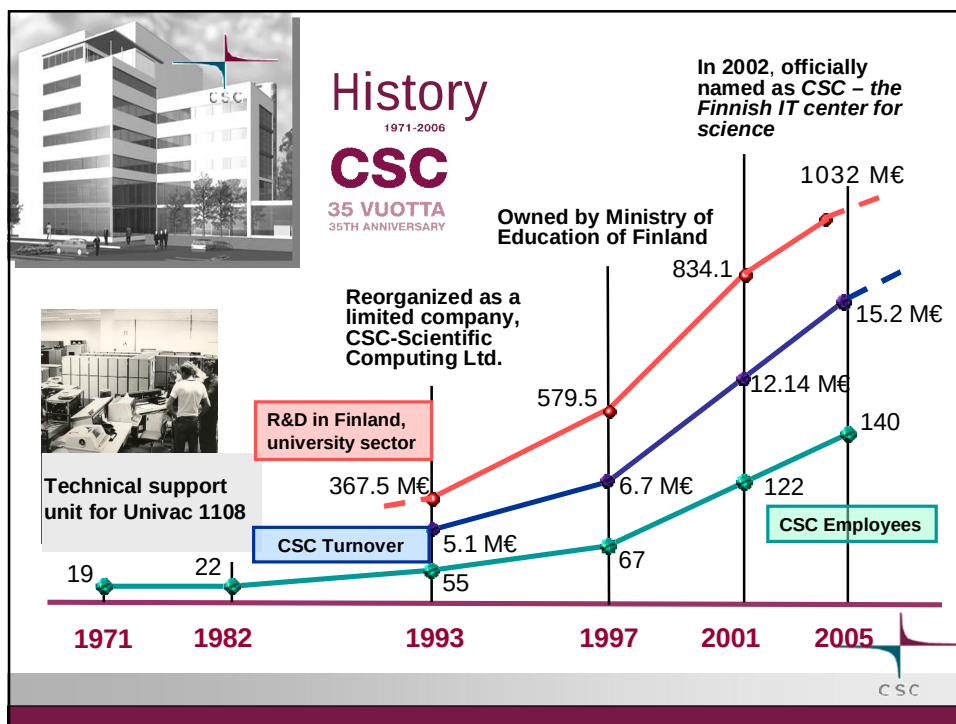
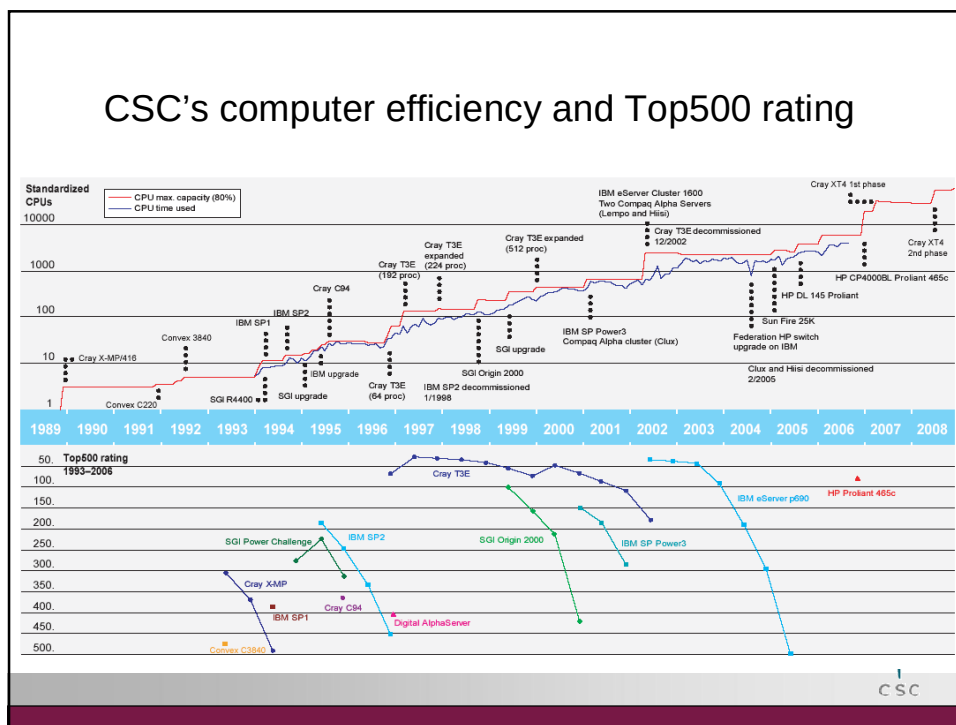


Who the heck is CSC?

CSC is, the Finnish IT center for science, administered by the Ministry of Education. CSC is a non-profit company providing IT support and resources for academia, research institutes and companies: modeling, computing and information services. CSC provides Finland's widest selection of scientific software and databases and Finland's most powerful supercomputing environment that researchers can use via the Funet network.



CSC



CSC's current supercomputer systems

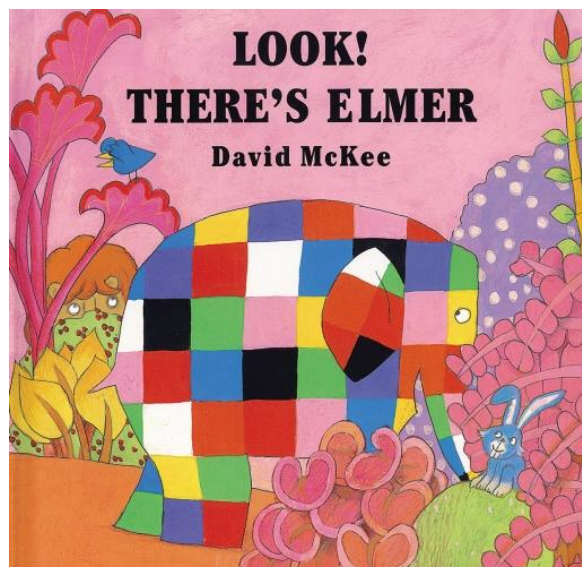
HP CP4000BL Proliant

- 10 TF peak performance
- 2048 compute cores
- AMD Opteron Dual Core 2.6 GHz
- 4 TB memory
- Infiniband interconnect
- RH EL 4 (Linux)



Cray Hood (XT4)

- 10.6 TF -> 70 TF peak
- initial phase: 2048 cores, 11 cabinets
- final phase: 6736 cores, 18 cabinets
- AMD Opteron Dual Core 2.6 GHz, Quad Core
- 1 GB/core memory
- Cray SeaStar 2 interconnect (3D torus)
- Unicos/lc (Linux, LWK Catamount in compute nodes)



Wikipedia:

[Elmer J.](#): Dj of the [DatDing! Dj Team](#) in the Netherlands, Europe. Hip-Hop and R&B DJ / Producer

[Elmer the Patchwork Elephant](#), the title character in a series children's picture books by David McKee

Elmer, a fictional bull, "husband" of [Elsie the Cow](#)

[Elmer Fudd](#), a Looney Tunes character

[Elmer Elephant](#), the titular character of a [Silly Symphonies](#) short

Picture taken from <http://www.randomhouse.co.uk>



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**
- **After the initial phase the development has been driven by applications**
 - MEMS, microfluidics, composite structures, optical fiber manufacturing, crystal growth, blood flow, Glaciology
- **Elmer includes a large number of physical models and modern numerical methods**



Elmer – Why?

- **An environment for making the expert services of CSC available for a larger number of customers**
 - Many researchers don't have their own code to start with
 - when a problem is solved, others can benefit
- **Way to keep up the knowhow**
- **An important tool for generating projects with external funding**
 - Tailored models for special needs
- **PR**
 - Free software efficient and well targeted advertisement



Elmer - Developers

➤ Current main developers

- CSC: Mikko Lyly, Mika Malinen, Juha Ruokolainen, Peter Råback, Thomas Zwinger

➤ Other/past developers & contributors

- CSC: Antti Pursula, Ville Savolainen, Erik Edelmann
- VTT: Martti Verho
- TKK: Jouni Malinen, Harri Hakula, Mika Juntunen, Mikko Byckling
- Trueflow: Ilkka Virkkunen
- Okmetic: Olli Anttila
- LGGE: Olivier Gagliardini
- etc...



Components of Elmer software suite

➤ Elmer actually is a suite of several programs

➤ You may use any of the components independently

➤ Preprocessing

- ElmerFront (MeshGen2D)
- ElmerGrid

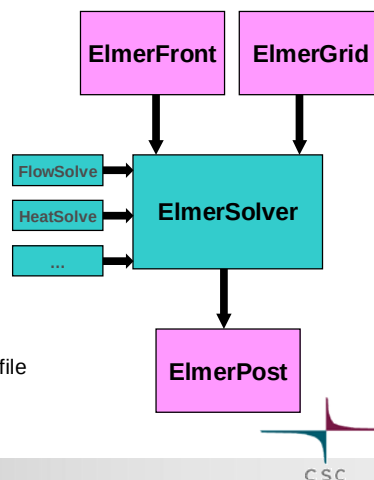
➤ ElmerSolver

➤ Post-processing

- ElmerPost

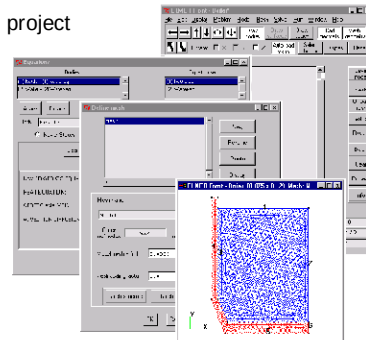
➤ Others

- MATC: library for on-the-fly arithmetics
- ElmerParam: black-box interfacing of ascii-file based simulations



ElmerFront

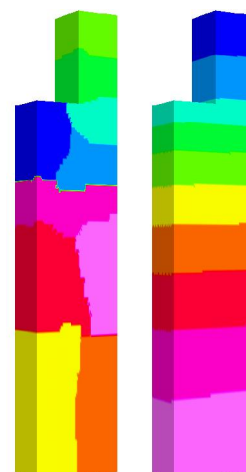
- **Graphical user interface of Elmer**
 - Developed by VTT as part of the initial project
 - Currently not further developed
- **Mesh generation**
 - 2D Delaunay mesh generation
- **Import of other formats**
 - Import of 2D/3D meshes
 - 2D CAD interface
- **Easiest tool for case specification**
 - Even educational use
- **Only basic solvers are supported through GUI**
 - Heat equation, Navier-Stokes, ...



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



ElmerSolver

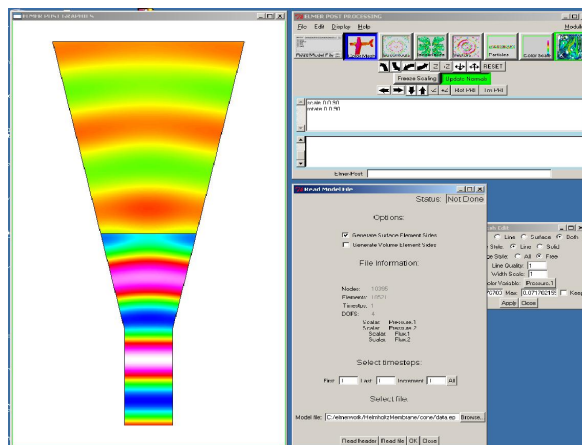
- **Assembly and solution of the finite element equation**
- **Partitioned operation with iterative solvers**
- **Note: When we talk of Elmer we mainly mean ElmerSolver**

```
> 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, iso-surfaces, vectors, particles
 - Animations
- **Includes MATC language**
 - Data manipulation
 - Derived quantities
- **Output formats**
 - ps, ppm, jpg, mpg



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 (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 Sham)
-



Elmer – numerical methods

- **Time-dependency**
 - Static, transient, Eigenmode analysis
- **Discretization**
 - Standard 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

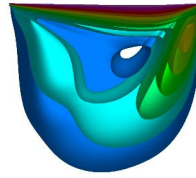
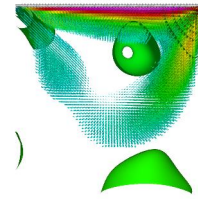


Parallel performance

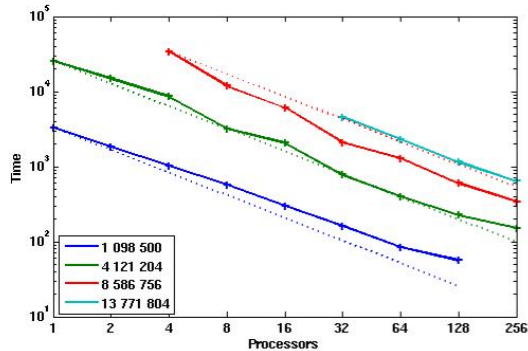
- Partitioning by Metis or simple geometric division
- Parallel assembly and solution by GMG or Krylov subspace methods.
- Parallel performance scales often well up to hundreds of processors
- Simulation with over one billion unknowns has been performed



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.



CSC

Elmer goes Open Source

- In September 2005 Elmer was published under Gnu Public License
- 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 advertisement 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>

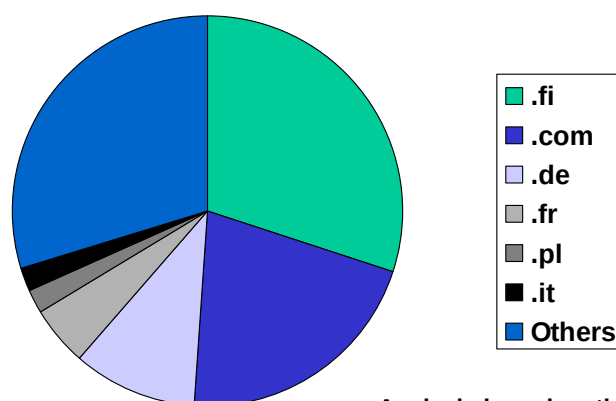


Fruits of Open Source publication

- **Increased popularity**
 - More than a thousand individual visitors on web-pages monthly
 - Significant number of heavy duty users in different application areas, for example computational glaciology community.
- **2nd hand distribution**
 - Available at Sun Grid for a price of 1 e/h
<http://www.network.com/>
 - Available in a computational engineering oriented Linux distro
<http://www.caelinux.com/CMS/>
 - Among the scientific software ported to FreeBSD
<http://www.freebsd.org/ports/science.html>
 - Ported to Mac by Trueflaw
 - Available via EGEE-grid
- **Increased popularity and visibility means new opportunities.**
 - Funding in national and EU-projects
 - Collaboration in different areas using Elmer as the platform



Elmer users by location



Analysis based on the
243 e-mail addresses
from the mailing lists
(9/2007)



Commercial exploitation of Elmer

- **Usage is free within GPL licensing**
 - Note: GPL has an "virus effect":
All products derived from GPL software must be published under GPL
- **As the owner of the code CSC may release the software under other licenses as well**
 - Commercial licensing allowing third party non-GPL software development
- **CSC has also withheld some software modules related to joint projects**
 - Parts may be added to GPL once the novelty value is used if agreed by all parties
- **Maintenance of full ownership to the code**
 - Joined Ownership Agreement



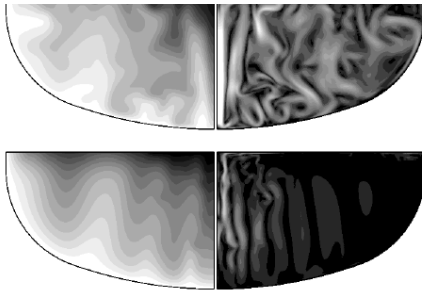
Elmer - Multiphysics capabilities

- **About 20 different physical models**
- **Iteration method is mainly used**
 - Consistency 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 consistent 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

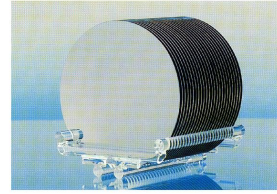


Czochralski Crystal Growth

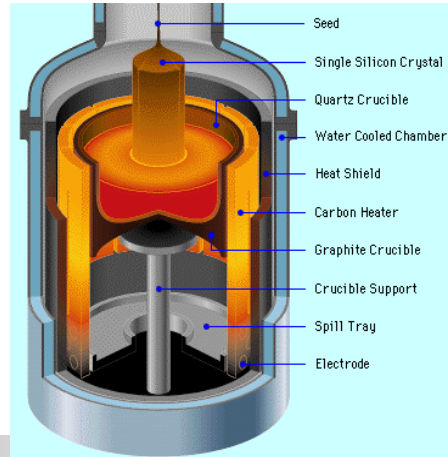
- Most crystalline silicon is grown by the Czochralski (CZ) method
- One of the key application when Elmer development was started in 1995



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



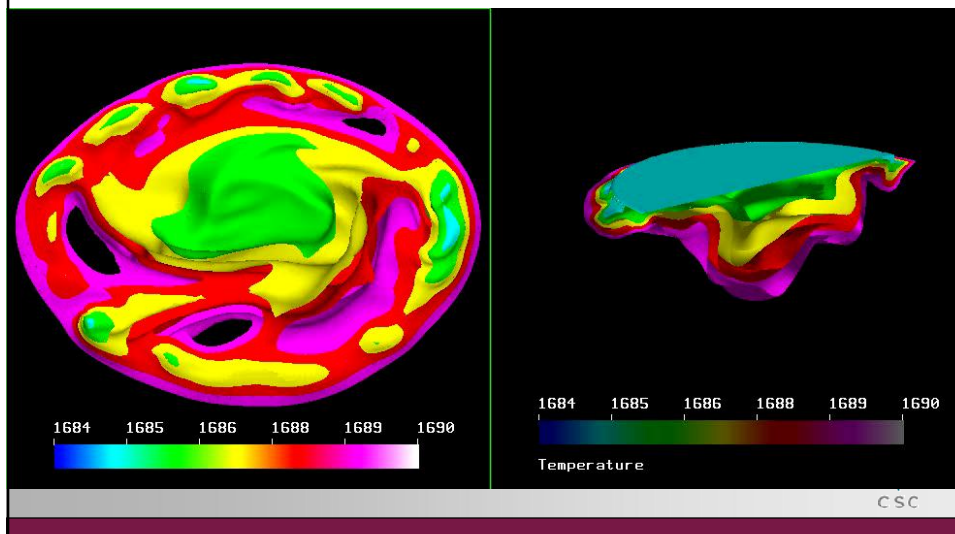
Figures by Okmetic Ltd.



CZ-growth: Transient simulation

Parallel simulation of silicon melt flows 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

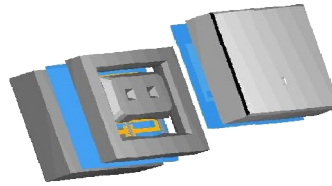
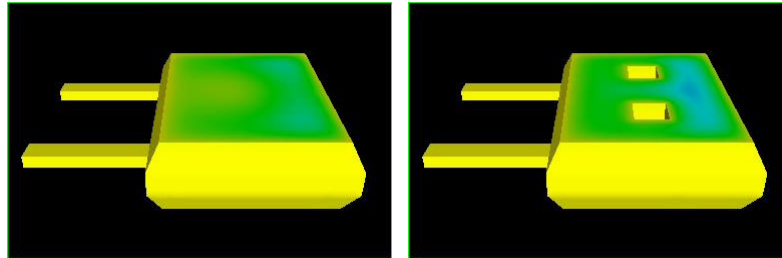


Figure by VTI Technologies

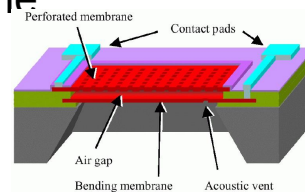
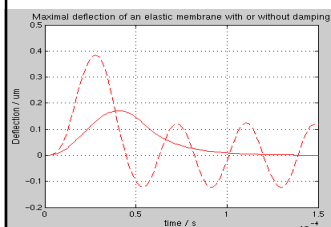
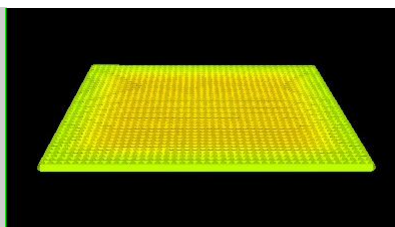
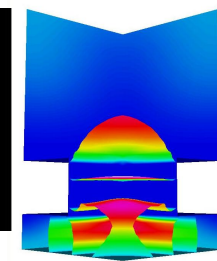


A. Pursula, P. Råback, S. Lähtenmäki and J. Lahdenperä, *Coupled FEM simulations of accelerometers including nonlinear gas damping with comparison to measurements*, J. Micromech. Microeng. **16** (2006), 2345-2354.



MEMS: Microphone membrane

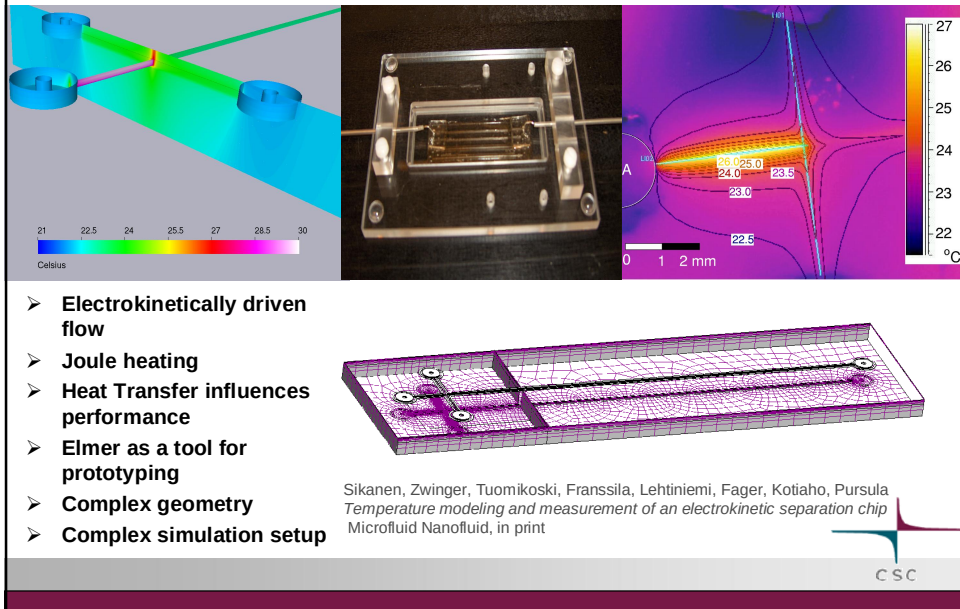
- MEMS includes often geometrical features that may be modeled with homogenization techniques
- Simulation shows the damping oscillations of a perforated micromechanical membrane



P. Råback et al., *Hierarchical finite element simulation of perforated plates with arbitrary hole geometries*, MSM 2003.

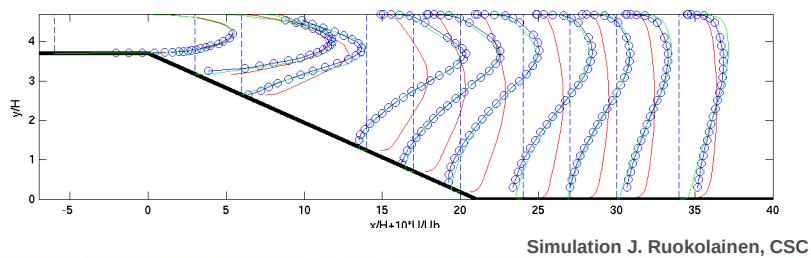
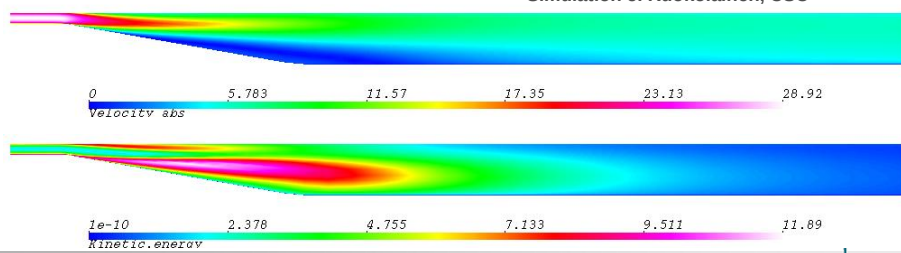


Microfluidics: Flow and heat transfer in a microchip



RANS Turbulence modeling

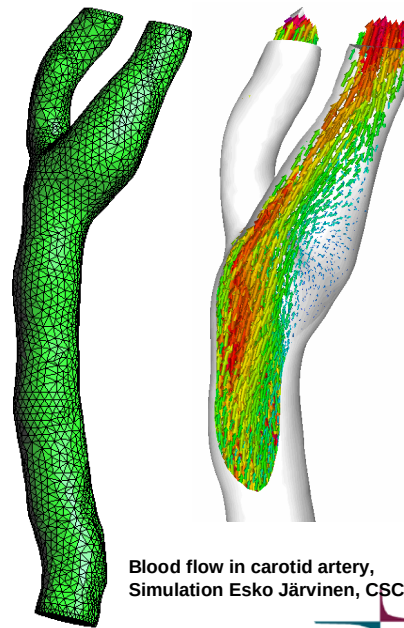
Comparison of $k-\varepsilon$ vs. ν^2-f –turbulence model (red & green line)



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)*

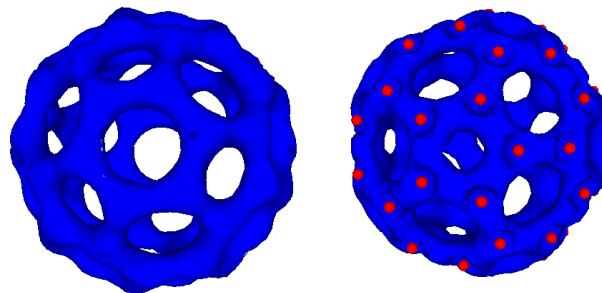


Blood flow in carotid artery, Simulation Esko Järvinen, CSC



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

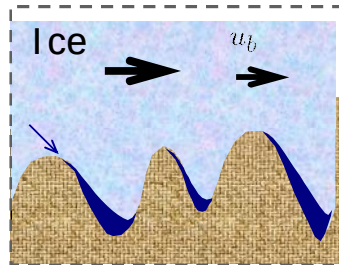


Simulation Mikko Lyly, CSC



Glaciology: Glaciers and Ice sheets

Water cavities under ice mass



O. Gagliardini, D. Cohen, P. Råback and T. Zwinger (2006)

Finite-element modeling of subglacial cavities and related friction law ,

J. Geophys. Res., 112

Glacier Flow

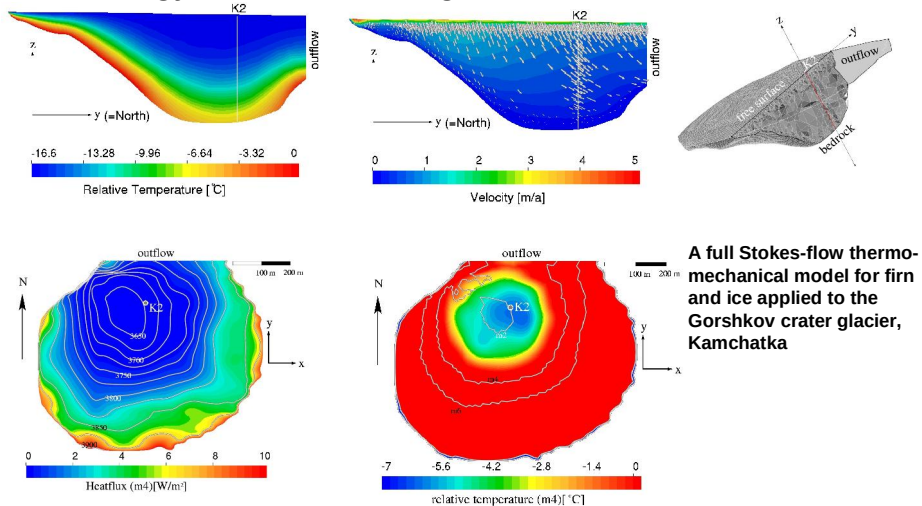
E. Le Meur, O. Gagliardini, T. Zwinger, J. Ruokolainen (2004)

Glacier flow modelling: a comparison of the Shallow Ice Approximation and the full-Stokes equation

C. R. Physique 5, 709-722



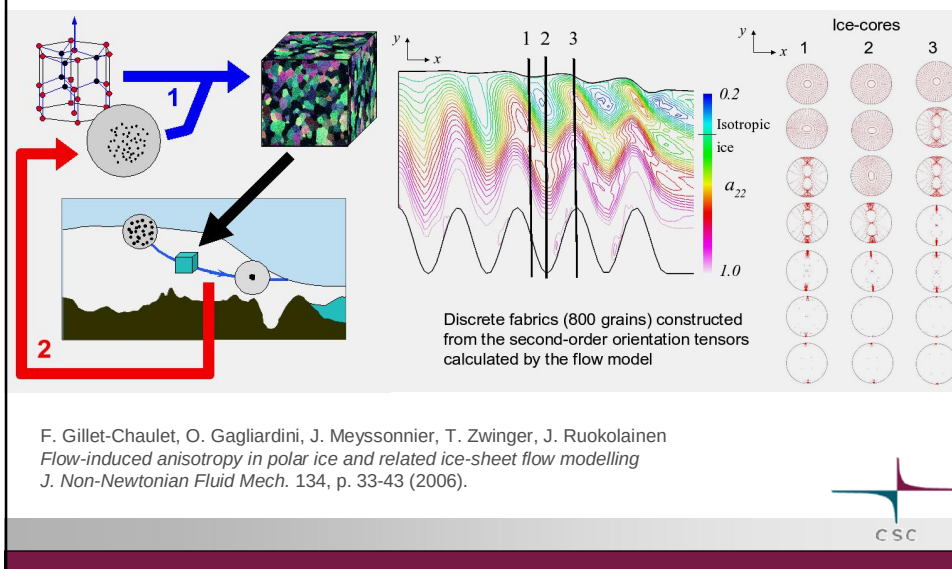
Glaciology: 3D Stokes of glaciers



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



Glaciology: Anisotropy of polar ice



Glaciology: Grand challenges

- Full Stokes simulations of continental size ice sheets
 = parallel runs of up to 100's of cores
- First attempts with GIS made by Zwinger & Greve

