Elmer Basic Course 25.5.

- 9.00-9.30 Registration & Coffee
- 9.30 I Session Welcome (all) Overview of Elmer Demonstration of ElmerGUI Instructions for the exercices
- 11.30 Lunch
- 12.15 II Session Guided exercices with simple walk-through examples in heat transfer, fluid dynamics, structural mechanics, electromagnetics, and in glasiology.
- 14.00 Coffee
- 14.20 III Session Using Elmer with other pre- and postprocessors (PR) Exercices continue Customizing ElmerGUI (ML)
- 16.30 End of day







Univac 1108 käyttöön 1971 1 prosessori 1 MB muistia huipputeho 0,093 Mflop/s oli aikanaan tehokas kone, mutta sitä ei kutsuttu supertietokoneeksi

CSC's supercomputers at the top500 list



Cray X-MP -käyttöön 1989 4 vektoriprosessoria -0.5 GB muistia -huipputeho 935 Mflop/s

Cray C94

-käyttöön 1995

-2 GB muistia

-4 vektoriprosessoria

-huipputeho 4 Gflop/s



CrayT3E -käyttöön 1997 -544 prosessoria -64 GB muistia -huipputeho 384 Gflop/s

SGI Origin 2000 -käyttöön 1998 -128 prosessoria -160 GB muistia -huipputeho 76,8 Gflop/s

IBM SP Power3 -käyttöön 2000 -128 prosessoria -64 GB muistia -huipputeho 192 Gflop/s



IBM p690 Power 4 -käyttöön 2002 -512 prossoria -512 GB muistia -huipputeho 2.2 Tflop/s



HP Proliant CP4000 BL -käyttöön 2007 -1024 prosessoria -4096 GB muistia -huipputeho 10,6 Tflop/s



Cray XT4 -käyttöön 2007 -1012 prosessoria -2024 GB muistia -huipputeho 10,5 Tflop/s

Cray XT4/XT5 -käyttöön 2008 - 2356 prosessoria - 10,3 Tb muistia -huipputeho 86,7 Tflop/s

Elmer - an Open Source Finite Element Software for Multiphysical Problems

Peter Råback CSC, Finnish IT Center for Science

> Elmer Basic Course 25th May 2010, CSC, Espoo

Outline

- Introduction to Elmer
 - As a project
 - As a software
- Elmer & Multiphysics
- Examples on Elmer usage

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 (2008-2010) 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

Fruits of Open Source publication

- Increased popularity
 - More than a thousand individual vistors on web-pages monthly
 - Significant number of serious users in different application areas, for example computational glasiology community.
- 2nd hand distribution
 - Several Linux distributions: Ubuntu, Debian and CAELinux
 - FreeBSD
 - Mac OS
 - Sun Grid (for a price of 1 e/h)
 - 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 @sf

Usage Statistics For Elmer-fem

Rank ~1000

Downloads
 ~1000 / month



elmerfem.org statistics 3/2010: continents



3 428 käyntiä 6 maanosasta

elmerfem.org statistics 3/2010: continents

Käynnit ? 3 428 % sivuston kokonaismäärästä: 100,00 %		Sivua/käyntikerta ? 5,47 Sivuston keskiarvo: 5,47 (0,00 %)	Keskim. aik sivustossa 00:05:1 Sivuston kes 00:05:15 (0,0	a ? 5 kiarvo: 00 %)	% uusia käyntejä 39,18 % Sivuston keskiarvo: 38,89 % (0,75 %)	?
	Tietojen tarkkuustaso: Maano	osa 🎸	Käynnit 🗸	Sivua/käyntiker	ta Keskim. aika sivustossa	
1.	Europe		2 384	5,5	56 00:05:27	
2.	Americas	668	5,4	41 00:04:19		
3.	Asia	306	4,8	88 00:05:00		
4.	Oceania	33	4,3	36 00:06:10		
5.	Africa		31	5,7	71 00:08:56	
6.	(not set)		6	12,8	83 00:16:09	

elmerfem.org statistics 3/2010: countries



3 428 käyntiä 66 maat ja alueet

	Tietojen tarkkuustaso: Maa tai alue 😆	Käynnit 🗸	Sivua/käyntikerta	Keskim, aika sivustossa
1.	Germany	468	5,85	00:05:19
2.	United States	419	5,36	00:04:06
3.	Finland	392	7,34	00:07:54
4.	Switzerland	290	6,83	00:07:36
5.	France	287	3,67	00:02:58
6.	United Kingdom	198	6,42	00:05:23
7.	Canada	162	6,13	00:05:22
8.	Italy	107	4,72	00:03:40
9.	Iran	101	4,04	00:03:11
10.	Russia	73	3,34	00:03:24
11.	Czech Republic	73	3,27	00:02:11
12.	Japan	70	6,54	00:05:40
13.	Netherlands	68	4,47	00:06:32
14.	Belgium	67	7,40	00:08:02
15.	Austria	64	4,73	00:07:42
16.	Poland	58	3,62	00:02:42
17.	Spain	57	4,96	00:03:01
18.	Slovakia	55	4,40	00:04:47
19.	Argentina	53	3,79	00:02:48
20.	India	37	3,62	00:03:17
21.	Australia	28	4,93	00:06:31
22.	China	26	7,81	00:09:56
23.	South Africa	25	6,76	00:10:47
24.	Sweden	25	3,32	00:01:21

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 HeatSolve 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

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 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 - Physical Models

- Heat transfer
 - Heat equation
 - Radiation with view factors
 - convection and phase change
- Fluid mechanics
 - Navies-Stokes (2D & 3D)
 - Turbulence models: k-ε, v²-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
 - Mainly steady-state and harmonic analysis
 - Edge-element formulation
- Electrokinetics
 - Poisson-Boltzmann
 - Poisson-Nernst-Planck
- Quantum mechanics
 - DFT (Kohn Scham)

Elmer - Numerical Methods

- Time-dependency
 - Static, transient, eigenmode, 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

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+ILUO. 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.



Coupling of physical phenomena

- Equations are inherently coupled and the coupling is explicitly shown in the equations
 - *E* and *B* in Maxwell's eq., *p* and *v* in Navier-Stokes eq.
- The different energy domains are coupled by a source or drain
 - viscous dissipation of kinetic energy to heat
- Coupling by material law
 - *v* and *T* by temperature dependent density
- Implicit coupling by the shape of the computational domain
 - large displacements and fluid flow

Some possible multiphysical combinations

Equation	Field	Т	V	Е, В	С	и
Energy	Temperature, T	-				
Navier-Stokes	Velocity, <i>v</i>	1	-			
Maxwell's	Electric & magnetic, <i>E, B</i>	2	3	-		
Diffusion, Reaction	Consentration, <i>c</i>	4	5	6	-	
Elasticity	Displacement, <i>u</i>	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

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





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

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

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.

Iterative vs. monolithic solution (analogy)

Let's assume that the equations are solved using Newton-Raphson iteration **Iterative solution**

$$\begin{cases} f_x dx^{(m+1)} &= -f(x^{(m)}, y^{(m)}) \\ g_y dy^{(m+1)} &= -g(y^{(m)}, x^{(m+1)}) \end{cases}$$

Monolithic solution

$$\begin{bmatrix} f_x & f_y \\ g_x & g_y \end{bmatrix} \begin{bmatrix} dx^{(m+1)} \\ dy^{(m+1)} \end{bmatrix} = -\begin{bmatrix} f(x^{(m)}, y^{(m)}) \\ g(y^{(m)}, x^{(m)}) \end{bmatrix}$$

- If the coupling is weak $(|f_x||g_y| >> |f_y||g_x|)$ the iteration method converges well
- The cross derivatives f_y and g_x may often be tricky determine. (for example, sensitivity of fluid flow to deformation)

Considerations on the iteration method

- Iteration method can easily be used when there are separate solvers for all equations
- Verification is straight-forward
 - Show consistancy (verify separate solvers) and reach convergence of coupled system
- Convergence may be poor
 - Under-relaxation may be used to improve convergence
 - Many new parameters to play with
- Often only conditionally stable (with respect to time-step)
- For simple equations it's much easier to design robust scalable methods
 - Multigrid

Considerations on the monolithic method

- Often difficult to implement
 - Implicit cross terms...
- Verification more tedious
- Ideal convergence
- Often real memory hogs
- Its difficult to find scalable linear algebra methods for the linear systems
 - Situation is manifested in parallel computing
 - Recent development: block preconditioners

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





Motivation for multi-scale approach

- The primary point of interest is the shape of the growth interface
 - The most relevant piece of information available
- The growth interface is a result of many time-scales
 - Global heat transfer has a time-scale of ~1h
 - Local velocity fluctuations have a stable time-scale of <1s
- Robust heating control only available in steady-state
 - In transient cases melting point is set
- Velocity fluctuations may not be accurately modeled with RANS models
 - Typically only a few convection rolls present
- We strive to combine the steady-state global heat transfer with ensamble averaged transient melt flow
 - Multi-scale approach

MEMS: Inertial sensor

- MEMS provides an ideal field for multiphysical 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.

MEMS: Microphone membrane

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





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

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)



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

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

Smoluchowski's temperature jump

$$T_{\rm G} - T_{\rm W} = \frac{2 - \sigma_T}{\sigma_T} \frac{2\gamma}{\gamma + 1} \frac{\lambda}{Pr} \frac{\partial T}{\partial n}$$





Simulation Moritz Nadler, 2008

Microfluidics: Flow and heat transfer in a microchip



- Electrokinetically driven flc^{*}
- 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 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-structureinteraction
- 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



Glaciology: 3D Stokes of glaciers



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

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



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 & green line)



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



VMS – Kelvin-Helmholtz instabilitv

- Instability occuring between flow layers
- Animation shows the development of the instability
- Computations carred out with the VMS model of Elmer
- Animation with two interfaces:



VMS - Rayleigh-Benard convection

- Instability initiated by a temperature difference
- Number of convection rolls is defined by the Rayleigh number
- With high enough Rayleigh numbers the flow is fully chaotic





VMS – Rayleigh-Benard convection

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AT		

Levelset method

2D levelset of a falling bubble









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

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

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
- Mikko.Lyly@csc.fi & Peter.Raback@csc.fi
 - Finnish university customers get the best support

Thank you for your attention!