Multiphysics simulation with Elmer examples with weak and strong coupling

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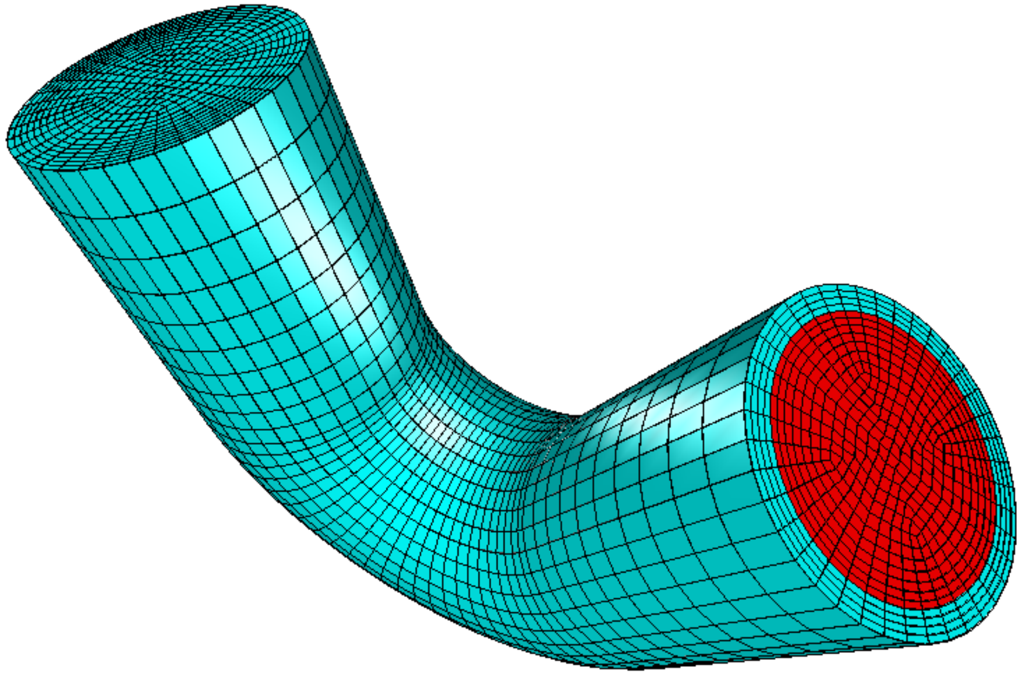
Classification of coupled problems

- Weak/loose vs. strong/tight coupling
  - May mean both physical or numerical coupling
- Continuous vs. discrete
  - Mainly matter of taste & implementation
- Coupling on bulk or boundary
  - Same mesh vs. different mesh
- Implicit or explicit coupling
  - Does the coupling appear as a field or via material law
- Same scale vs. different scale
  - Coupled problems often multiscale problems
- Same method vs. different method
  - Homogeneous vs. heterogeneous/hybrid

Coupling of flow & heat



This is the ElmerGUI totorial
Thermal Flow in a curved pipe
in ElmerTutorials.pdf

- Solid pipe (iron) wall filled with fluid (water)
- Hot (350 K) inflow on one end of the pipe and cold (300 K) outside of the pipe

$$\rho\, c\,(\partial T/\partial t + \boldsymbol{u}\cdot\nabla T) = \nabla\cdot(\kappa\nabla T) + \rho\sigma$$

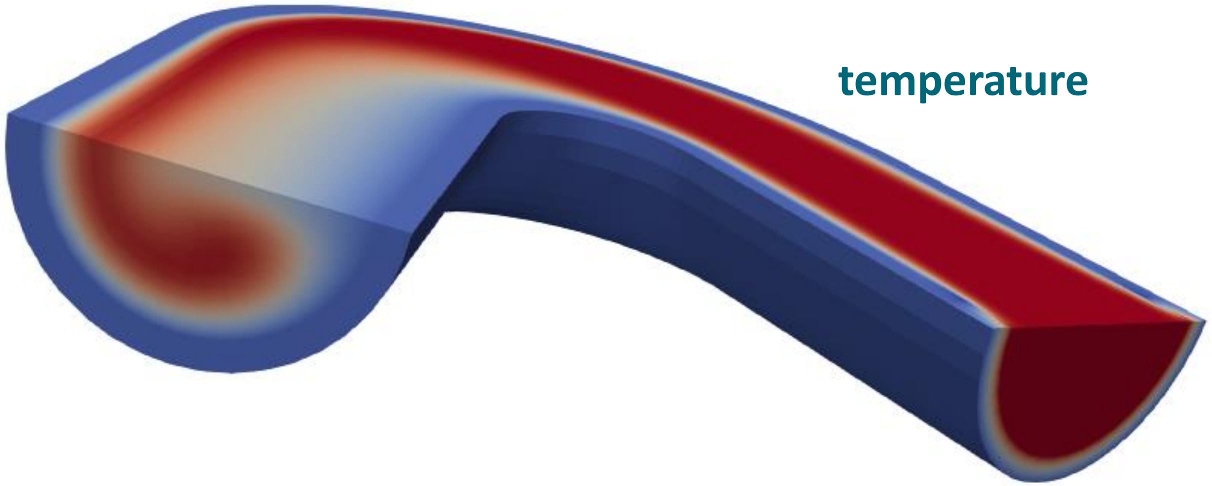
$$\rho\,(\partial \boldsymbol{u}/\partial t + \boldsymbol{u}\cdot\nabla \boldsymbol{u}) = -\nabla\, p + \nabla\cdot(\mu\dot{\boldsymbol{\epsilon}}(\boldsymbol{u})) + \rho\boldsymbol{f}$$

- Inherent coupling via velocity
- Potential coupling via material laws

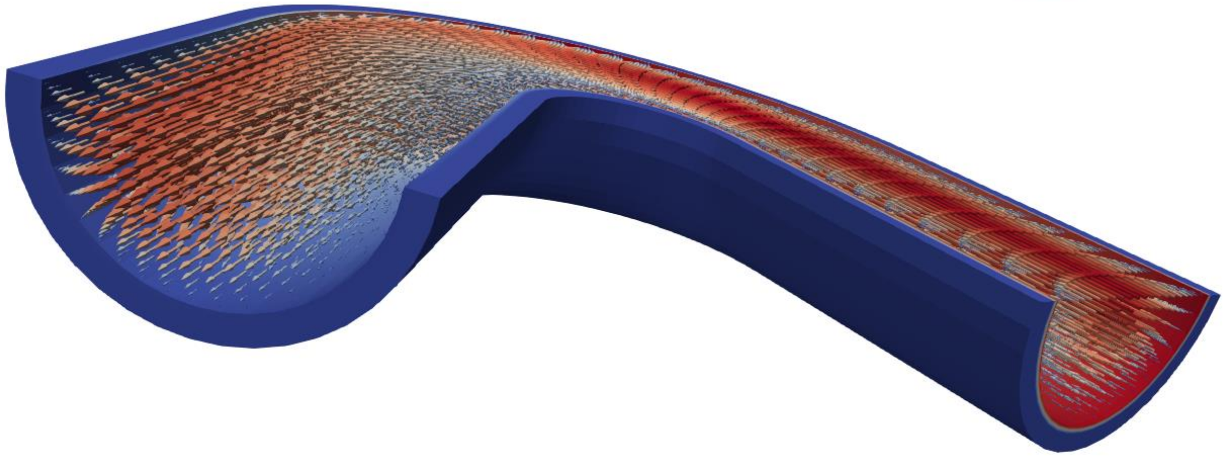
Coupling of flow and heat – hiararchical coupling

- Assuming material parameters constant we have one-directional coupling
  - Hierarchical coupling
- Only one steady-state iteration is needed
  - Order of equations must be correct!
  - Navier-Stokes -> Heat

```
Material 1
  Name = "Water (room temperature)"
  Viscosity = 1.002e-3

Simulation
  Steady State Max Iterations = 1
```



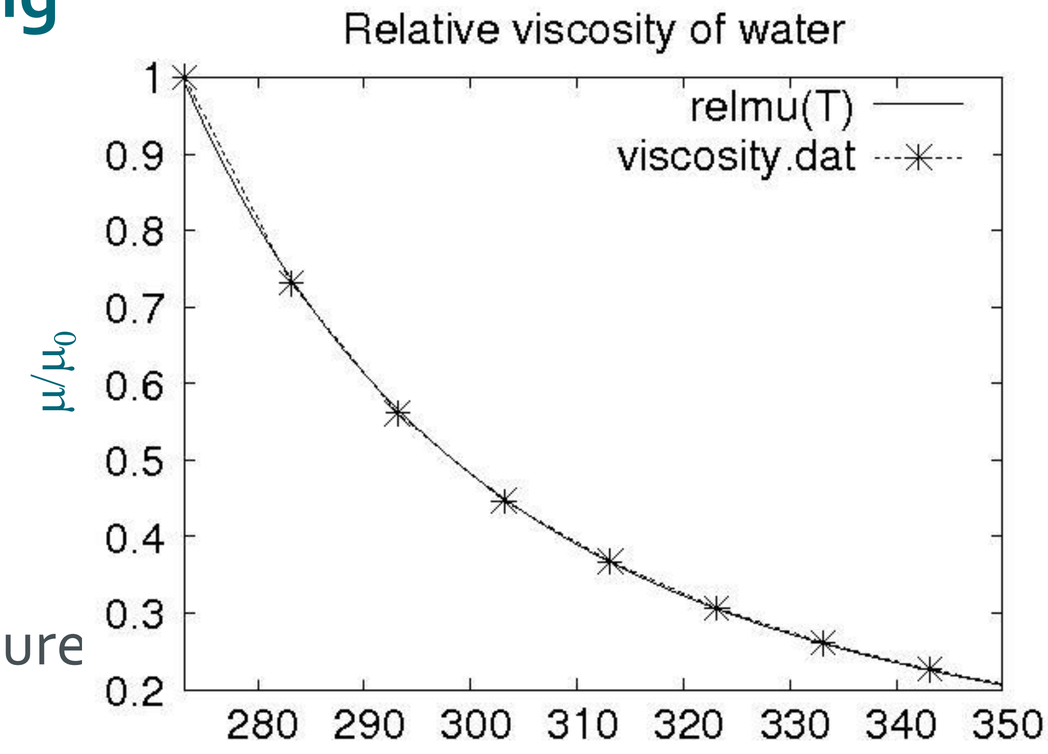
temperature



wall pressure + velocity vectors

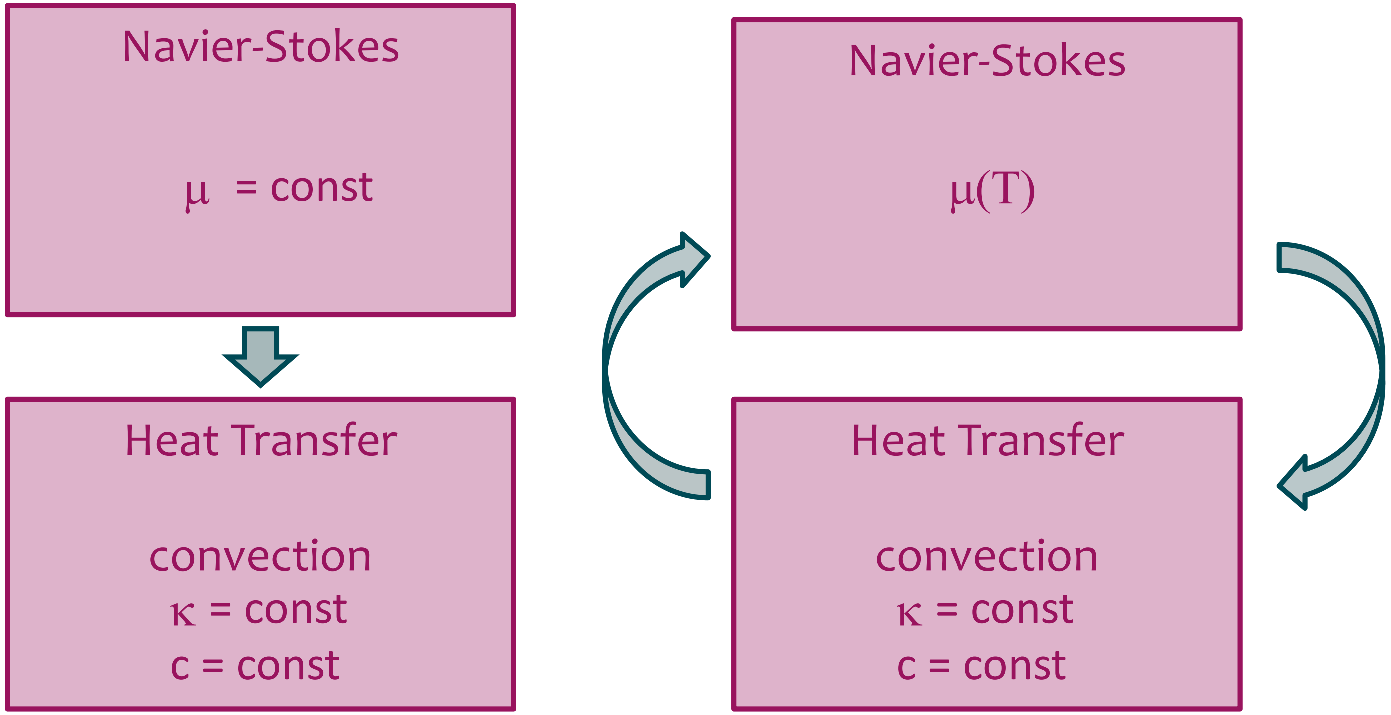
Coupling of flow and heat – weak coupling

- Assuming temperature-depedent material parameters we may introduce backcoupling
  - Temperature depedent viscosity
- Most real valued keywords in Elmer may be functions of anything
- Let us create viscosity as a function of temperature
  - Table
  - MATC
  - LUA
  - **Fortran routine**
- We also need to add coupled system iterations!



$$\mu = \mu_0 \exp(-1.704 \; -5.306 \; 273.15/T + 7.003 \, (273.15/T)^2)$$

Coupling of flow and heat – hierarchical vs. loose coupling

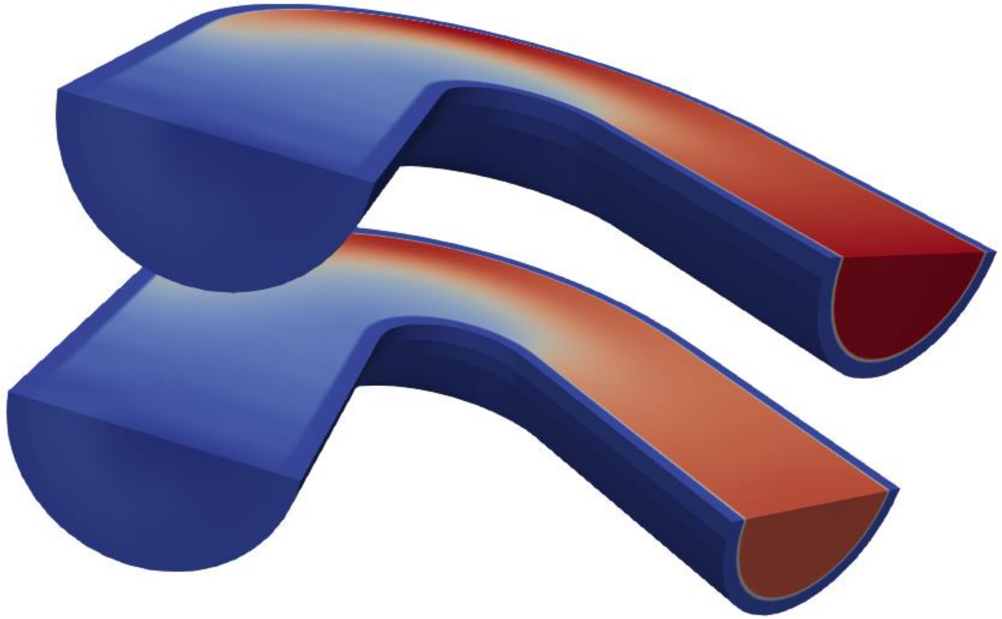


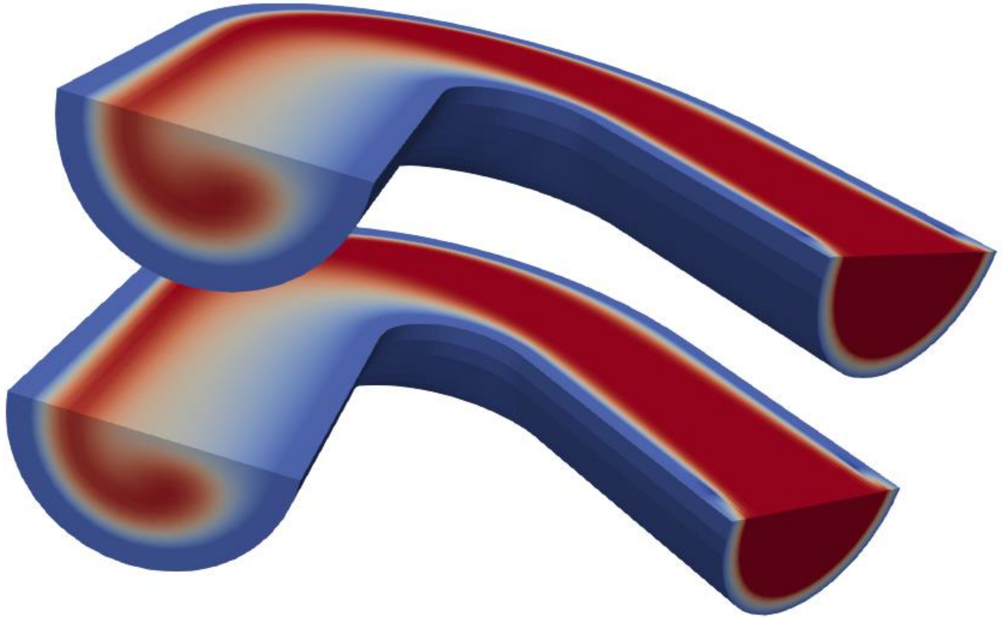

```
FUNCTION WaterViscosity
  USE DefUtils
  IMPLICIT NONE
  TYPE(Model_t) :: Model
  INTEGER :: n
  REAL(KIND=dp) :: temp, visc
  REAL(KIND=dp), PARAMETER :: a=-1.704_dp, &
     b=-5.306_dp, c=7.003_dp, visc0 = 1.788d-03
  REAL(KIND=dp) :: z

  IF( temp <= 0.0_dp ) &
    CALL Fatal("WaterViscosity","Invalid temp value")

  z = 273.15/temp
  visc = visc0 * EXP(a + b*z + c*(z**2))

END FUNCTION WaterViscosity
```

```
Steady State Max Iterations = 50

Viscosity = Variable “temperature”
  Procedure “WaterFuncs” “WaterViscosity”
```

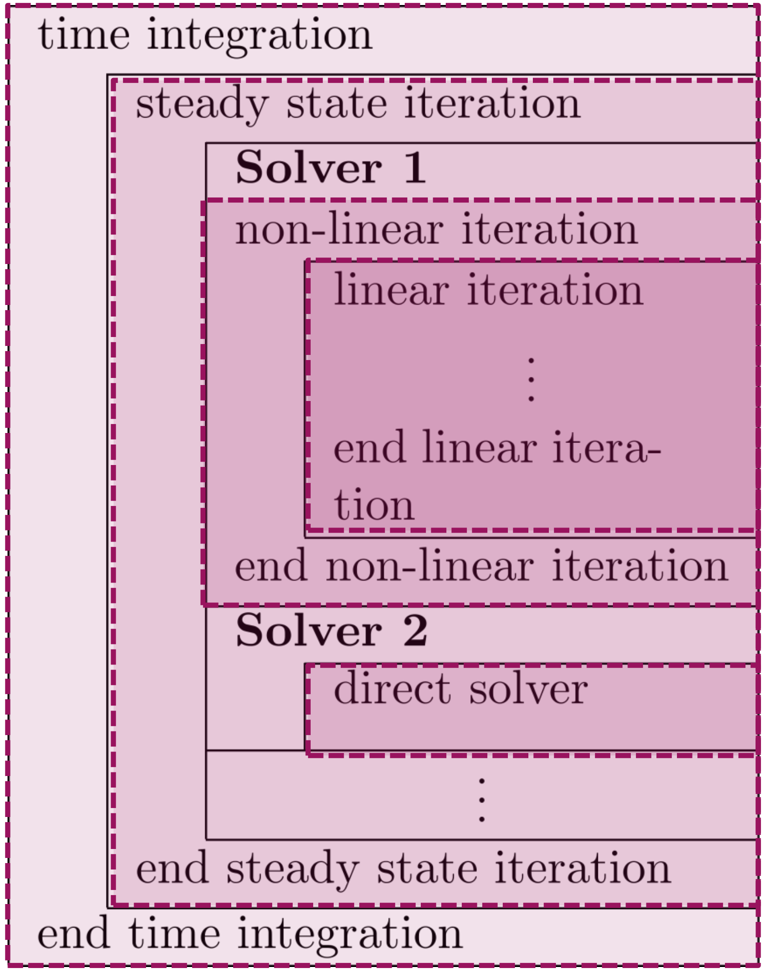
Coupling of flow and heat – weak coupling

- For this case loosely coupled iteration converges nicely
  - The effect on viscosity variation is very moderate (barely visible for the eye)
  - Just a few iterations needs
- Driving force is forced convection
  - Not affected by change in viscosity
- More challenging if the driving force is directly linked to the other equation
  - E.g. natural convection
    (convection caused by temperature dependent density)





Nested iterations in Elmer as defined by the SIF file



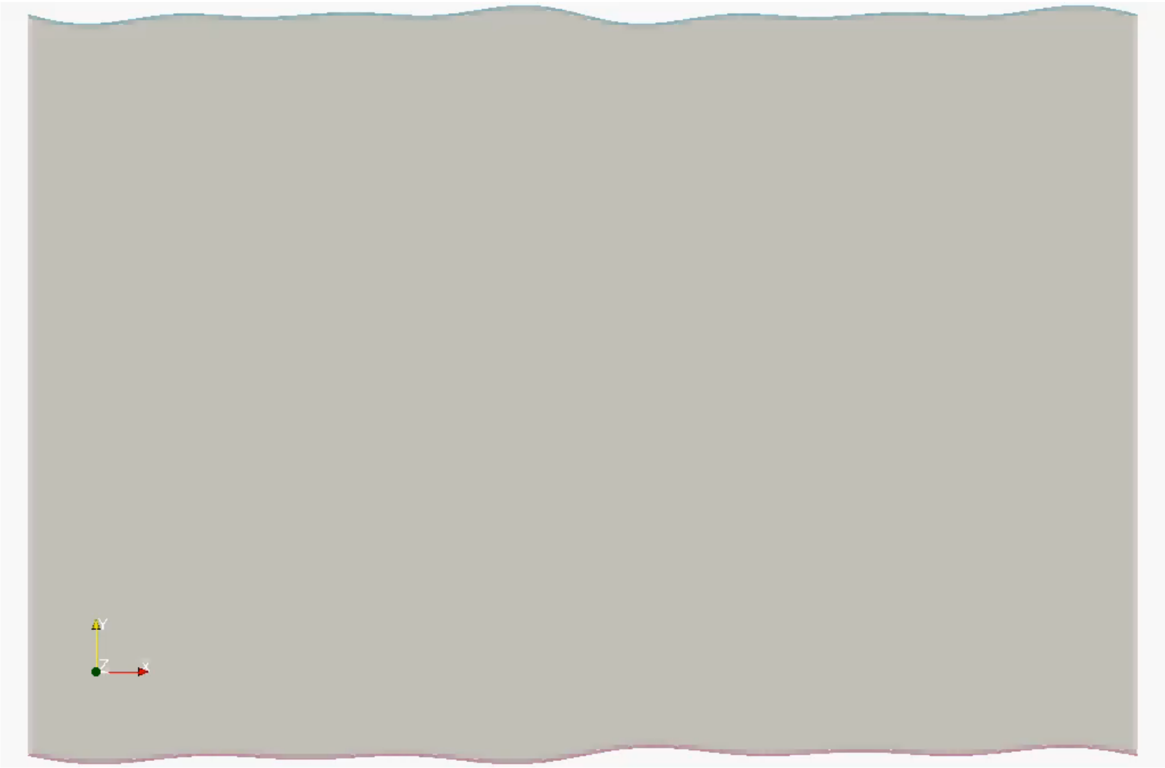
1. `Timestep Intervals`
2. `Steady State Max Iterations`
3. `Nonlinear Max Iterations`
4. `Linear System Max Iterations`
4. `Linear System Convergence Tolerance`
3. `Nonlinear System Convergence Tolerance`
2. `Steady State Convergence Tolerance`
1.

Coupling of flow and heat – strong physical coupling

- Natural convection
  - Same equations, density assumed to depend on temperature

$$\rho = \rho_0(1 - \beta(T - T_0))$$

- Physical coupling is strong
  - Driving force is caused by the temperature dependent density
- Weak numerical coupling usually ok
  - Decreasing timestep helps to stabilize the iteration
  - There isn't even a stationary solution with high enough temperature difference
- Test cases: **NaturalConvection***



Time harmonic Navier-Stokes equations – strong numerical coupling

- In dissipative acoustics (e.g. mobile phones) we have strong physical coupling between pressure and temperature via ideal gas law

- Linearized Navier-Stokes equations in frequency domain

$$i\omega\rho_0\vec{v} + \frac{(\gamma-1)C_V\rho_0}{\beta T_0}\nabla T - (\lambda + \mu - \frac{i(\gamma-1)C_V\rho_0}{\omega T_0\beta^2})\nabla(\nabla\cdot\vec{v}) - \mu\Delta\vec{v} = \rho_0\vec{b},$$ **momentum**

$$-\kappa\Delta T + i\omega\rho_0 C_V T + \frac{(\gamma-1)C_V\rho_0}{\beta}\nabla\cdot\vec{v} = \rho_0 h.$$ **energy**

$$\rho = \frac{i\rho_0}{\omega}\nabla\cdot\vec{v}.$$ **continuity**

- It is very hard to reach convergence with loose coupling
  - Monolithic matrices are needed

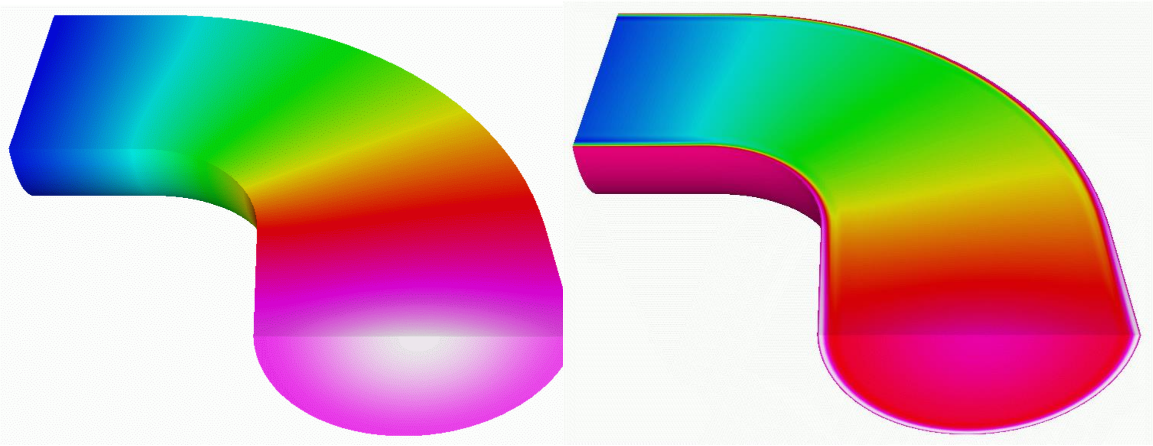
- See "**AcousticsSolver**" in Elmer ModelsManual

Solving time-harmonic Navier-Stokes equations

- Unfortunately the monolithic matrix equation turns out to be very difficult for stanard linear solvers
  - High condition number
  - Direct solvers used with limited success
- Instead a complicated but robust block preconditioning scheme needed to be created
  - Block Gauss-Seidel procedure applied using the lower diagonal system
  - The problem is further moved to finding optimal linear solvers for the subproblems
- Same principles later applied to Stokes

M. Malinen, Boundary Conditions in the Schur Complement Preconditioning of Dissipative Acoustic Equations. SIAM J. Scientific Computing. 29. 1567-1592, 2007.

$$\begin{bmatrix} C & D & 0 & 0 & L_U \\ E & J & 0 & 0 & 0 \\ H_P & H_\Theta & M_W & 0 & 0 \\ 0 & 0 & L_W & R & 0 \\ 0 & 0 & 0 & N & M_U \end{bmatrix} \begin{bmatrix} P \\ \theta \\ W \\ Q \\ U \end{bmatrix} = \begin{bmatrix} G \\ 0 \\ 0 \\ F \\ 0 \end{bmatrix}$$



Pressure and temperature fields of acoustics field. Notice the temperature boundary layer.

Multiphysical prototype problem

- Assume two coupled problems where F is primarily related to x, and G to y. Solution is obtained from the system of equations $F(x,y) = 0$ and $G(y,x) = 0$. The main algorithmic coupling choices are:
- Hierarhical coupling: $$F(x) = 0 \\ \Rightarrow G(y,x) = 0$$
- Loose coupling: $$\begin{cases} F(x,y) = 0 \\ G(y,x) = 0 \end{cases}$$
- Tight coupling : $$\begin{pmatrix} F(x,y) \\ G(y,x) \end{pmatrix} = 0$$

Numerical solution using tight coupling

- Formally we can find the solution by Newton's method

$$\begin{bmatrix} x_{i+1} \\ y_{i+1} \end{bmatrix} = \begin{bmatrix} x_i \\ y_i \end{bmatrix} - \begin{bmatrix} F_x(x_i, y_i) & F_y(x_i, y_i) \\ G_x(y_i, x_i) & G_y(y_i, x_i) \end{bmatrix}^{-1} \begin{bmatrix} F(x_i, y_i) \\ G(y_i, x_i) \end{bmatrix}$$

- Solution in tight coupling would involve evalution of the Jacobian
  - Cross terms F_y and G_x may be difficult to estimate
  - Often inexact Newton methods are used
- In practice the inverse of the Jacobian is never formed

Solution using loose coupling

- Formally we find the solution iteratively from

$$\begin{cases} x_{i+1} & = & x_i - F_x^{-1}(x_i, y_j)\, F(x_i, y_i) \\ y_{i+1} & = & y_i - G_y^{-1}(y_i, x_{i+1})\, G(y_i, x_{i+1}) \end{cases}$$

- Loose coupling can be shown[1] to converge if

$$\|F_x^{-1}\|\, \|G_y^{-1}\|\, \|F_y\|\, \|G_x\| \leq 1$$

- For transient problems we can usually find a small enough timestep that this condition is met (conditionally stable)

1) Whiteley et. al. (2011), *Error bounds for block Gauss-Seidel solutions of coupled multiphysics problems*, Int. J. for Num. Meth. in Eng. 88(12), 1219-1237.

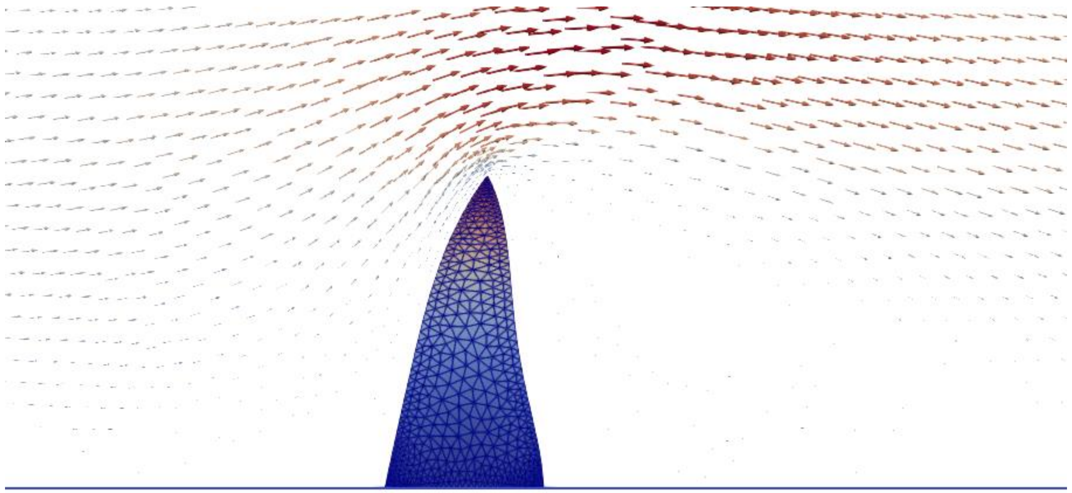
FSI – weak coupling

- Fluid-Structure Interaction (FSI) is a canonical multiphysics problem
  - FlowSolver & ElasticSolve
- Equality of forces
  - Fluid applies forces to structure
- Equality of velocities
  - Structure sets velocity to fluid
- Two ways to set force condition
  - Continuous – coded in ElasticSolver
  - Discrete – utilizes library functionality for nodal forces
- Exterior flow problems usually simple to solve with weak coupling
  - Very rigid objects lead to one-directional coupling

$$f_{solid} = -f_{fluid}$$

Test case: **fsi_beam_nodalforce**
Setting FSI conditions on the discrete level

Displacement 1 Load = Opposes "Flow Solution Loads 1"
Displacement 2 Load = Opposes "Flow Solution Loads 2"



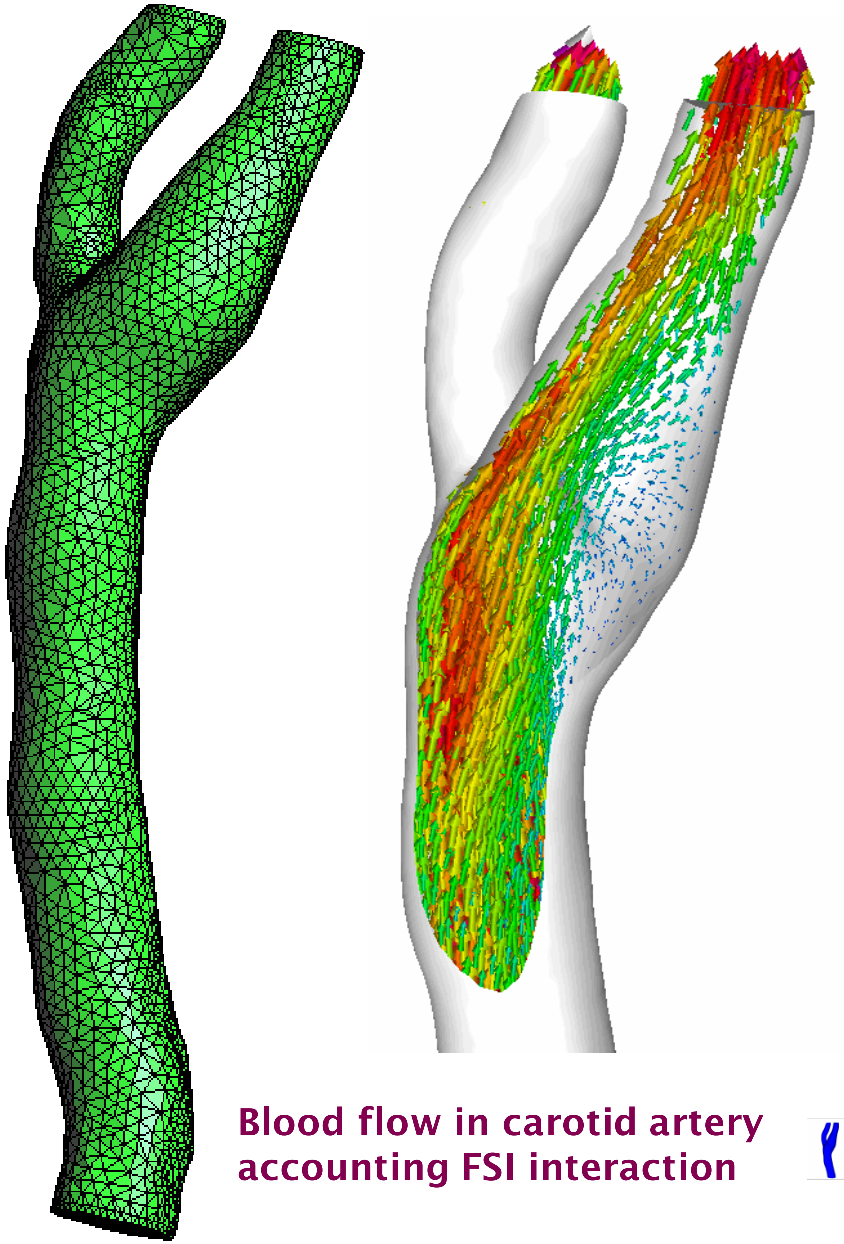
Test case: **fsi_beam**
Setting FSI internally on continuous level

Fsi Bc = True

FSI - 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

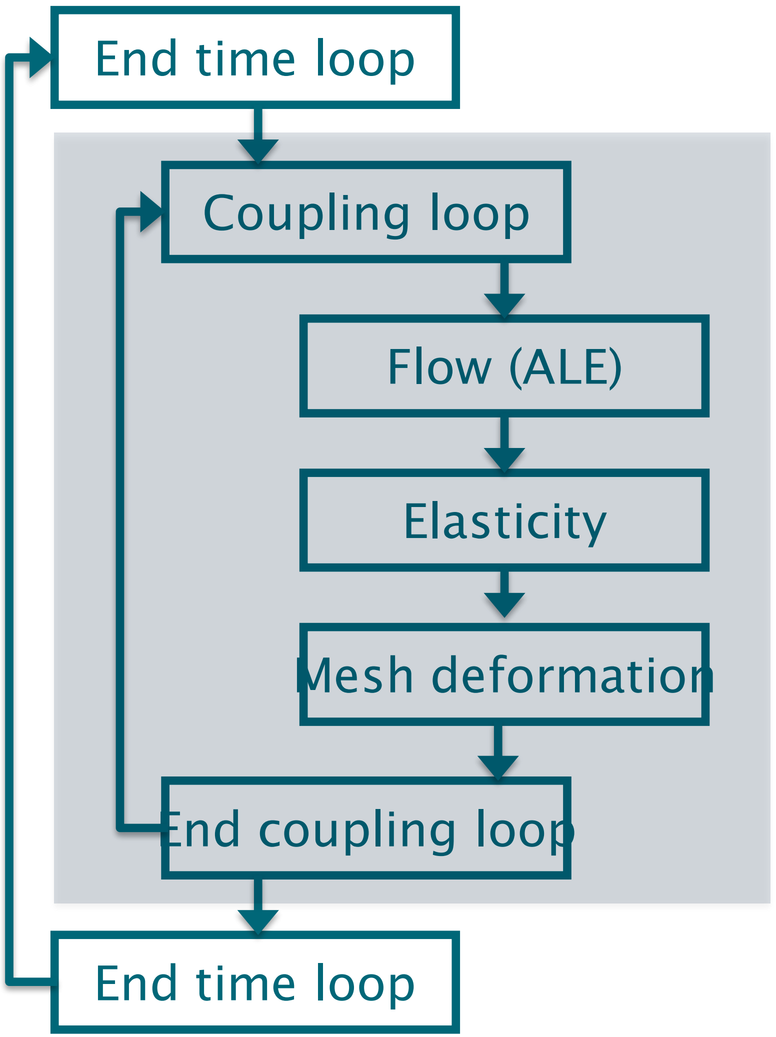
E. Järvinen, P. Råback, M. Lyly, J. Salonius. *A method for partitioned fluid-structure interaction computation of flow in arteries. Medical Eng. & Physics*, **30** (2008), 917-923



Blood flow in carotid artery accounting FSI interaction

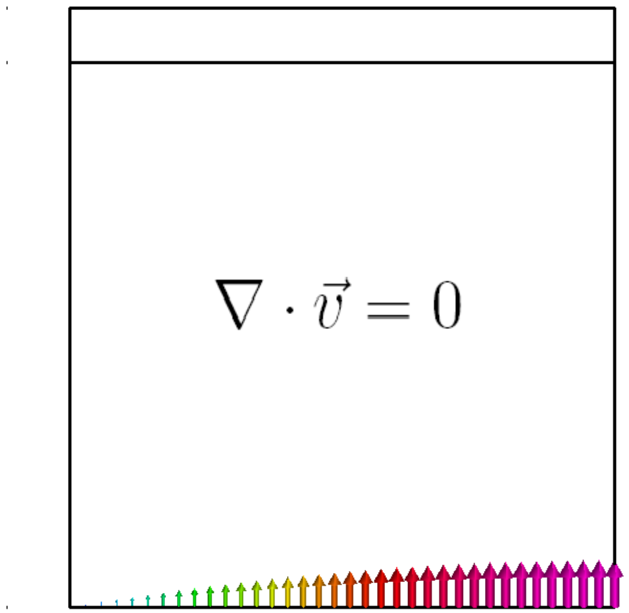
Loosely coupled FSI scheme

- Solve the **flow** problem
  - Velocity of structure used as BC on FSI boundary
- Solve the **structural** problem
  - Pressure traction used as force on FSI boundary
- Extend the **mesh** smoothly for the fluid domain
  - ALE discretization for the flow
- Continue until convergence is obtained
- Usually fails for arterial FSI



FSI - Failure of the loose coupling

- Imagine a closed elastic container filled with incompressible fluid
  - Initially the fluid is at rest and the velocity profile is defined at the inlet
- The continuity equation cannot be solved as there is a net flux into the domain
  - The coupled problem is still well posed!
- For semiclosed domains the pressure is over-estimated
  - Canonical example: arterial flow simulations
- Suggested remedy:
  modification of the continuity equation
  $\Rightarrow$ artificial compressibility (AC)



Modified continuity equation for internal FSI

- Determine the sensitity of the fluid volume of to pressure

$$C = \frac{1}{\delta P}\frac{\delta V}{V}$$

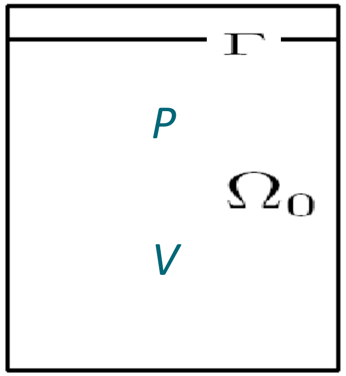
- Derive an equation of state for the fluid so that it can accomodate the same relative volume with the same pressure change

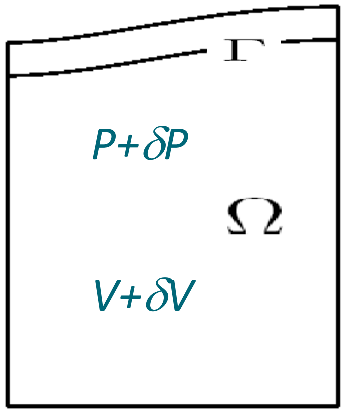
$$\frac{\delta\rho}{\rho} = C\,\delta P$$

- Modify the continuity equation respectively using compressibility as an iteration trick between consecutive FSI-iterations: ACM

$$\frac{C}{\Delta t}\left(p^{(m)} - p^{(m-1)}\right) + \nabla \cdot \vec{v}^{(m)} = 0$$

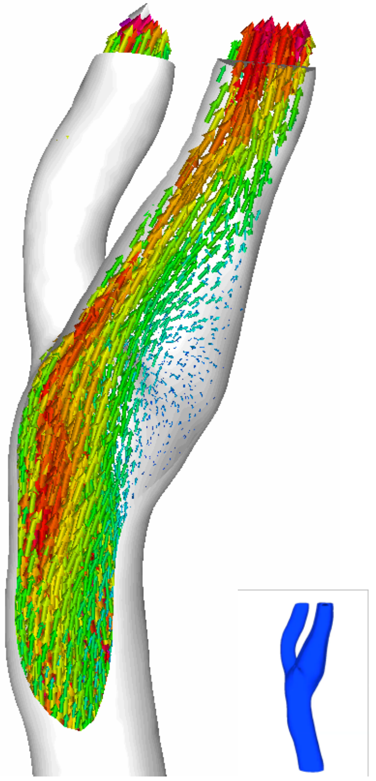
- Consistant with the original equation when convergence is reached!



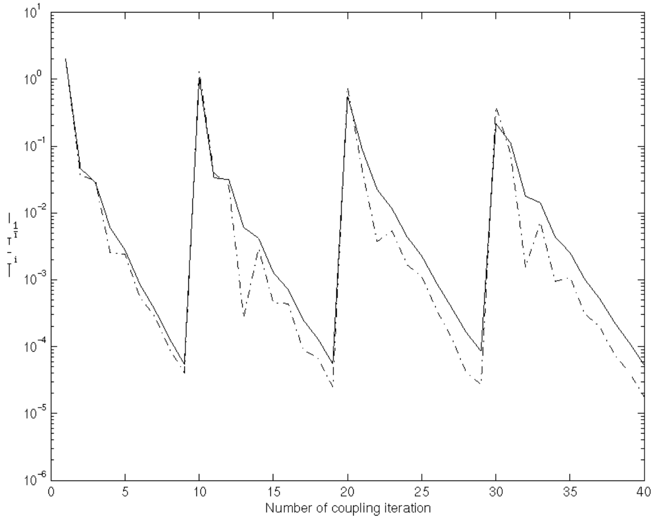


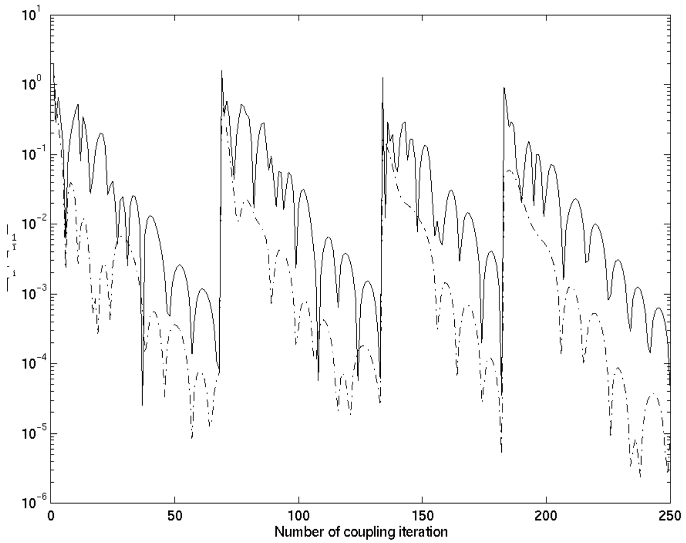
Artificial compressibility in FSI

- Artificial compressibility (AC) is used to enhance the convergence
- An optimal AC field may be defined by applying a test load to the strcucture and computing the relative **elemental volume change** per pressure unit[1]
- Convergence in the artery case is monotonic and rather fast
- Without the AC convergence is slow and cannot be guaranteed



Blood flow in carotid artery (Esko Järvinen, CSC)

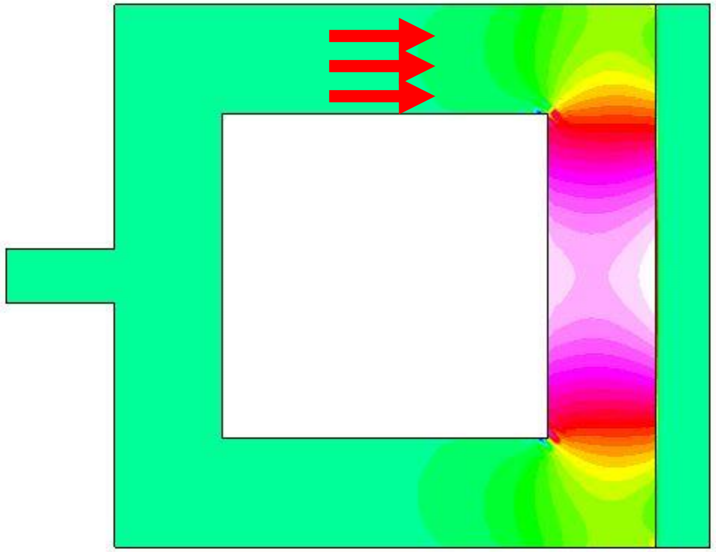




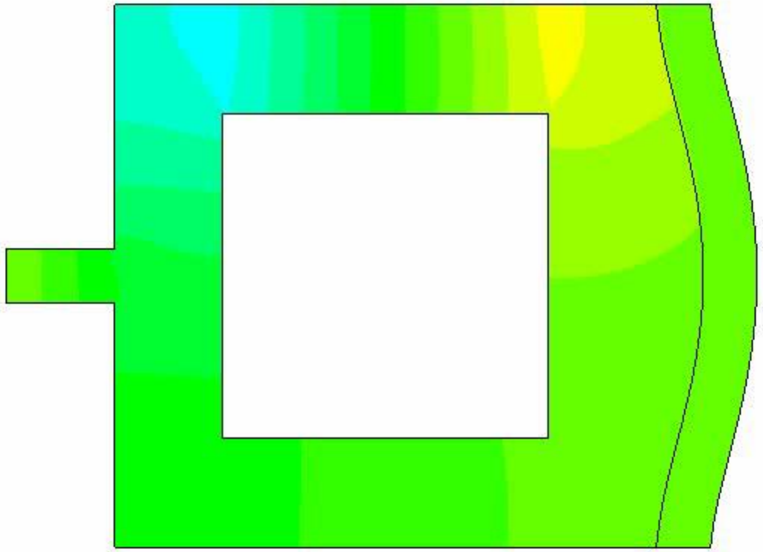
E. Järvinen, P. Råback, M. Lyly, J. Salonius. *A method for partitioned fluid-structure interaction computation of flow in arteries. Medical Eng. & Physics,* ***30*** *(2008), 917-923.*

FSI with articifical compressibility

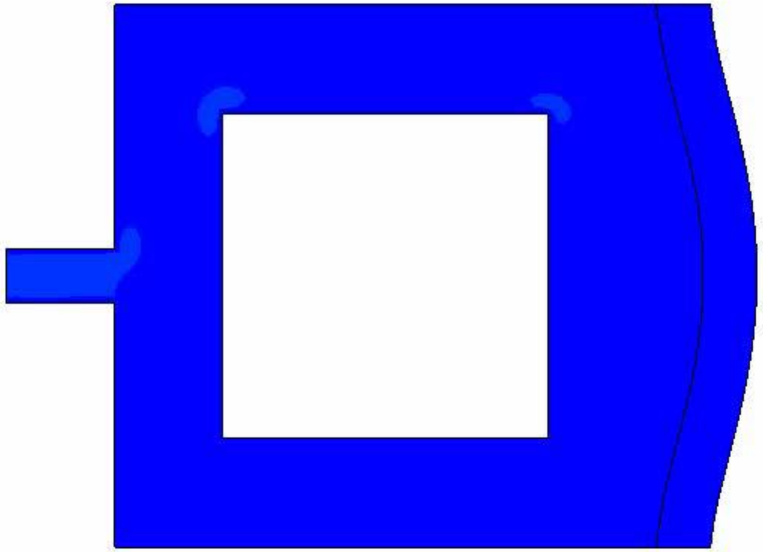
- Flow is initiated by a constant body force at the left channel
- Natural boundary condition is used to allow change in mass balance
- An optimal artificial compressibility field is used to speed up the convergence of loosely coupled FSI iteration



AC



Pressure

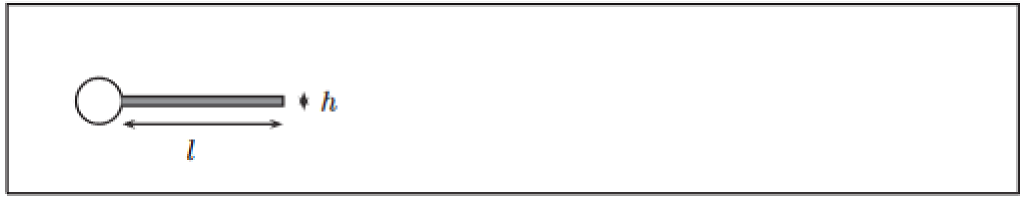


Velocity

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

FSI – Need for strong numerical coupling

- For transient cases convergence is usually obtained by loosely coupled schemes
- There are some cases where the coupling fails
  - E.g. case of Stefan Turek
    (Proposal for Numerical Benchmarking of Fluid–Structure Interaction Between an Elastic Object and Laminar Incompressible FlowUsually solved by strongly coupled schemes)



- In Elmer we have developed strongly coupled methods related to harmonic FSI problems
  - Solved in frequency range or as eigenvalue problems
  - Linear models for structure: plate, shell & solid
  - Linearized models for flow: e.g. Helmholtz equation

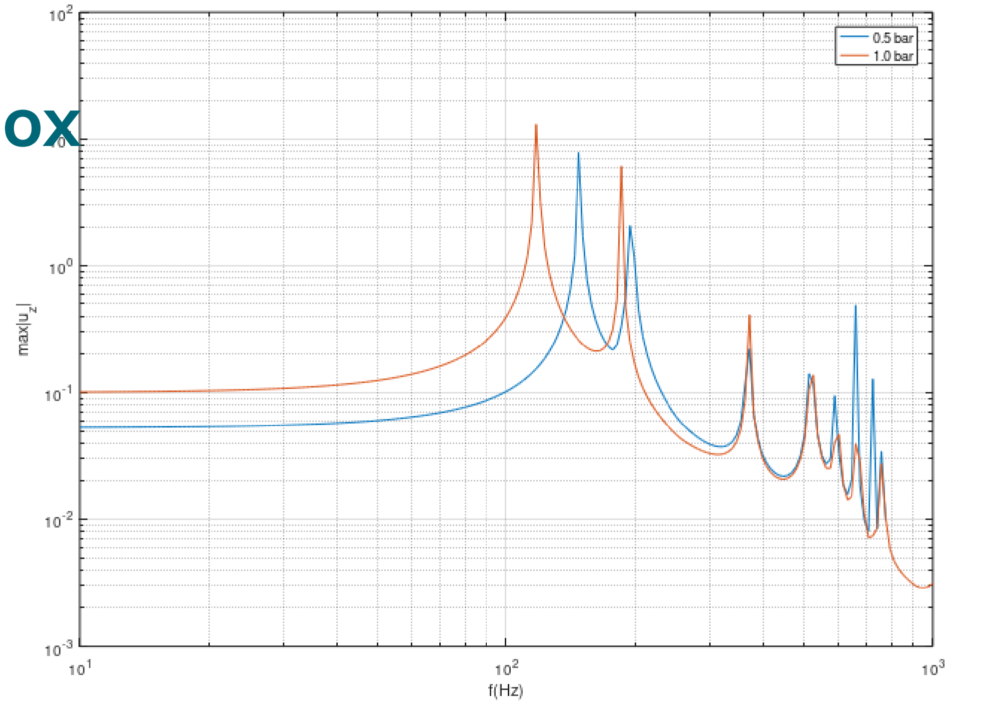
Strong FSI coupling of linear models

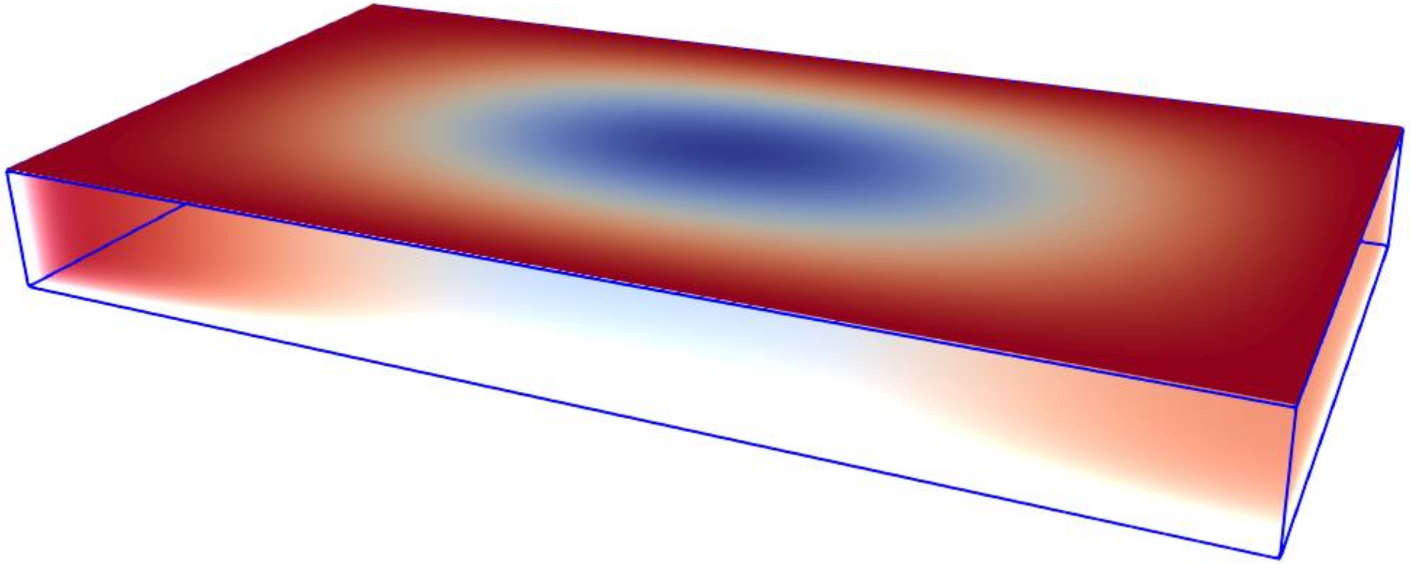
- Use standard models for fluid (*F*) and structure (*S*)
- One solver is the ”master”
  - The other solver acts as ”slave” only assembling its own matrix
- Library functionality is used to generate coupling matrices
  - How does fluid affect the structure: equality of forces (P_{sf})
  - How does structure affect fluid: equality of velocity/displacement
- Resulting matrix equation may be solved
  - Block techniques
  - Monolithic (only possibility for eigenvalue probelms)
- Tons of test cases: Shoebox*

$$\begin{pmatrix} S & P_{sf} \\ P_{fs} & F \end{pmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

Strong FSI coupling of linear models – shoebox

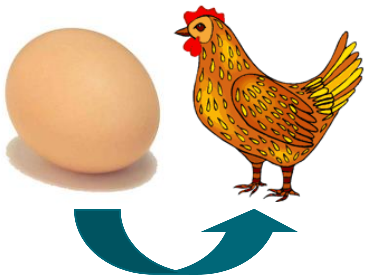
- Top of a "shoebox" is assumed to be a plate
- Inside of air is modeled using Helmholtz equation
- Basically equation is setup as monolithic but solved with block preconditioning
- How does the gas pressure affect the Eigenmodes?
- Test case: **ShoeboxFsiHarmonicPlate**



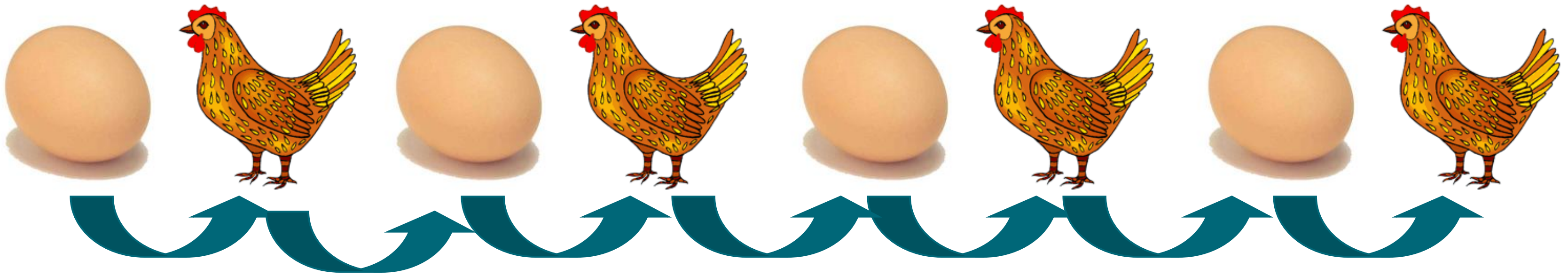


Solution strategies for coupled problems

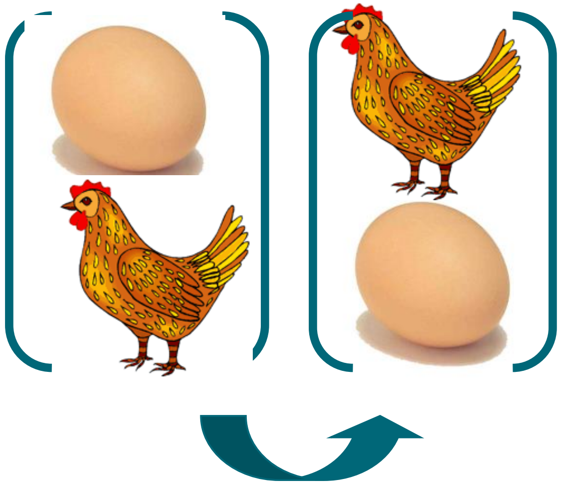
hierarchical coupling



loose coupling

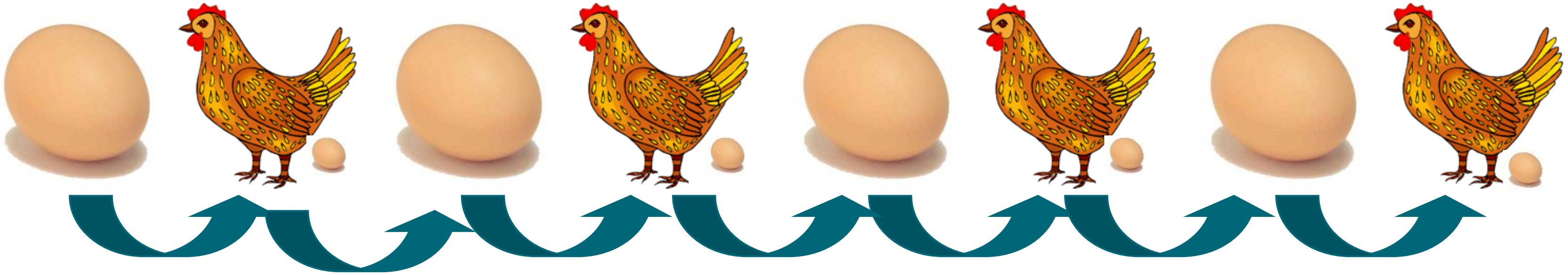


tight coupling

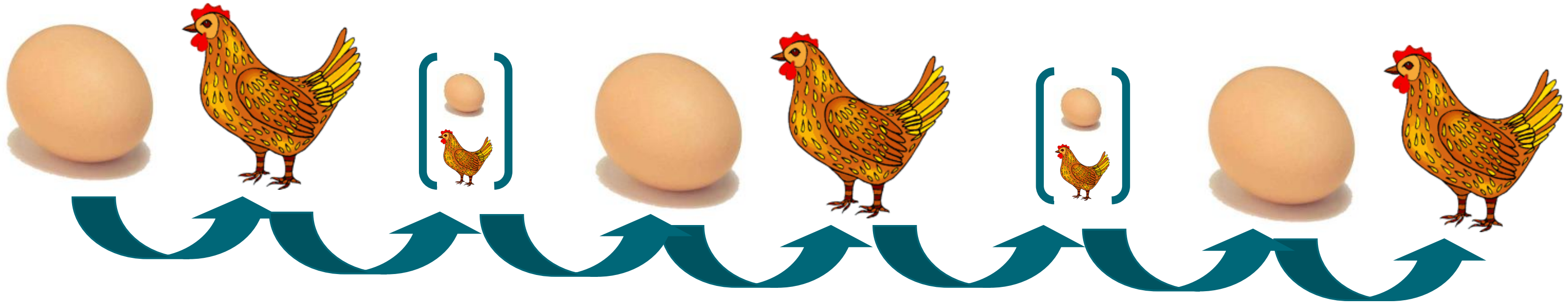


Tricks for improving the loose coupling method

Exchange additional information between models



Use on-the-fly lumped models to scale suggested fields



Li-Ion battery – multiscale problem

- System of four PDE's
- Electrolyte (macroscale)
  - 1D, 2D or 3D model
  - Poisson equation for the electrostatic potential accounting for ions
  - Transport equation for the ions
- Solid phase (microscale)
  - 1D model in spherical symmetry
  - Poisson equation for the electrostatic potential
  - Transport equation for the ions
- **For each node** of the electrolyte mesh we solve 1D equation for the solid phase

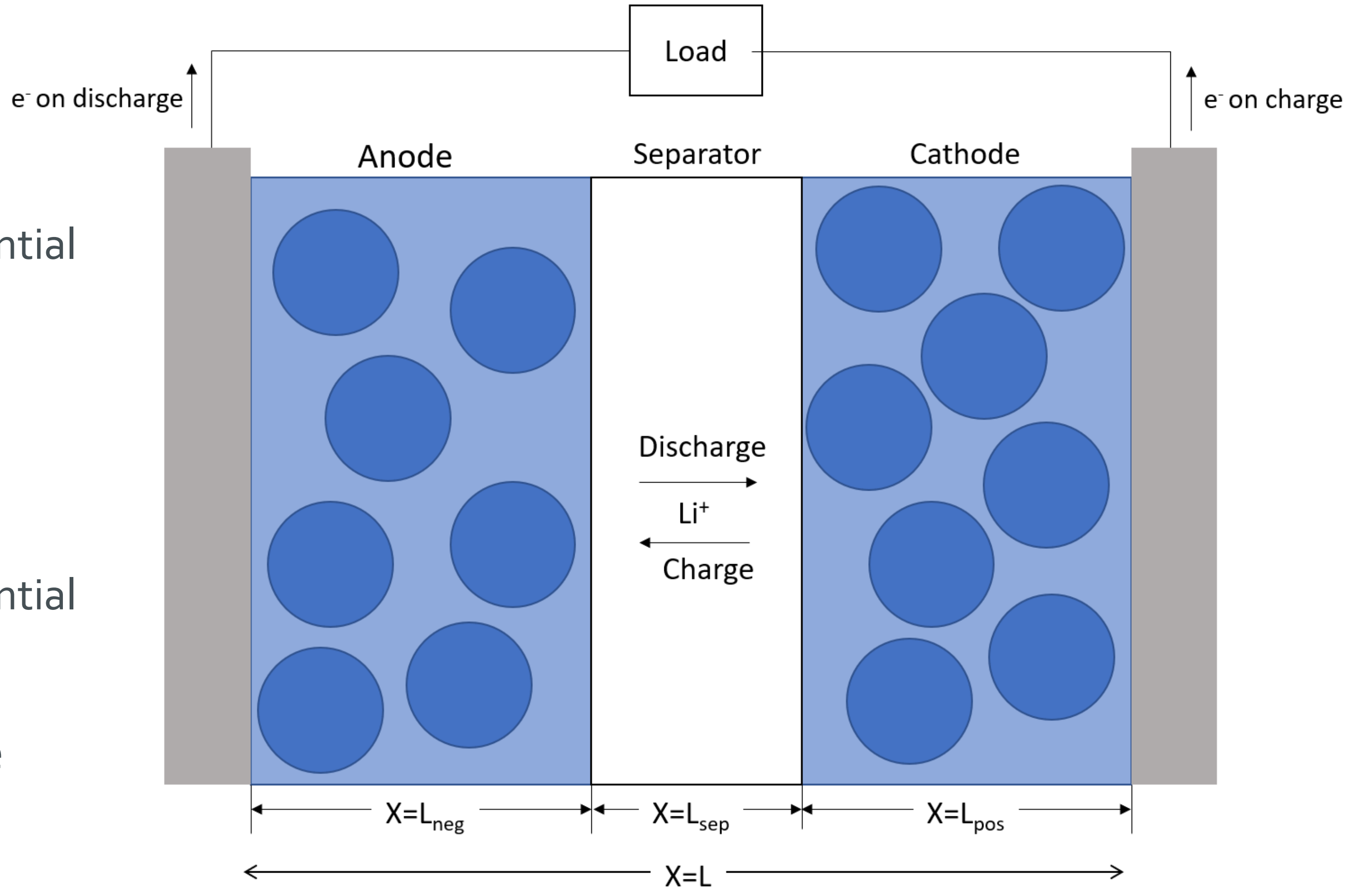


Figure: Timo Uimonen, Univ. Of Vaasa, 2020

Lithium-Ion battery – loosely coupled iteration

- Electrolyte and solid phase fluxes are determined by the hideously nonlinear Butler-Volmer equation

$$J_{Li} = a_s i_0 \left[\exp\left(\frac{\alpha_a F}{RT} \eta \right) - \exp\left(\frac{\alpha_c F}{RT} \eta \right) \right]$$

where the flux depends on potentials, e.g.

$$\eta = \varphi_s - \varphi_e - U,$$

$$U_n(x) = 8.0029 + 5.0647\, x - 12.578\, x^{\frac{1}{2}} - 8.6322e\text{-}4\, \frac{1}{x} + 2.1765e\text{-}5\, x^{\frac{3}{2}} - 0.46016\, \exp(15(0.06 - x)) - 0.55364\, \exp(-2.4326(x - 0.92))$$

- Multiscale nature suggests that only iteration method is realistic to implement
- Even with Newton's linearization >~100 nonlinear iterations often needed ;-<

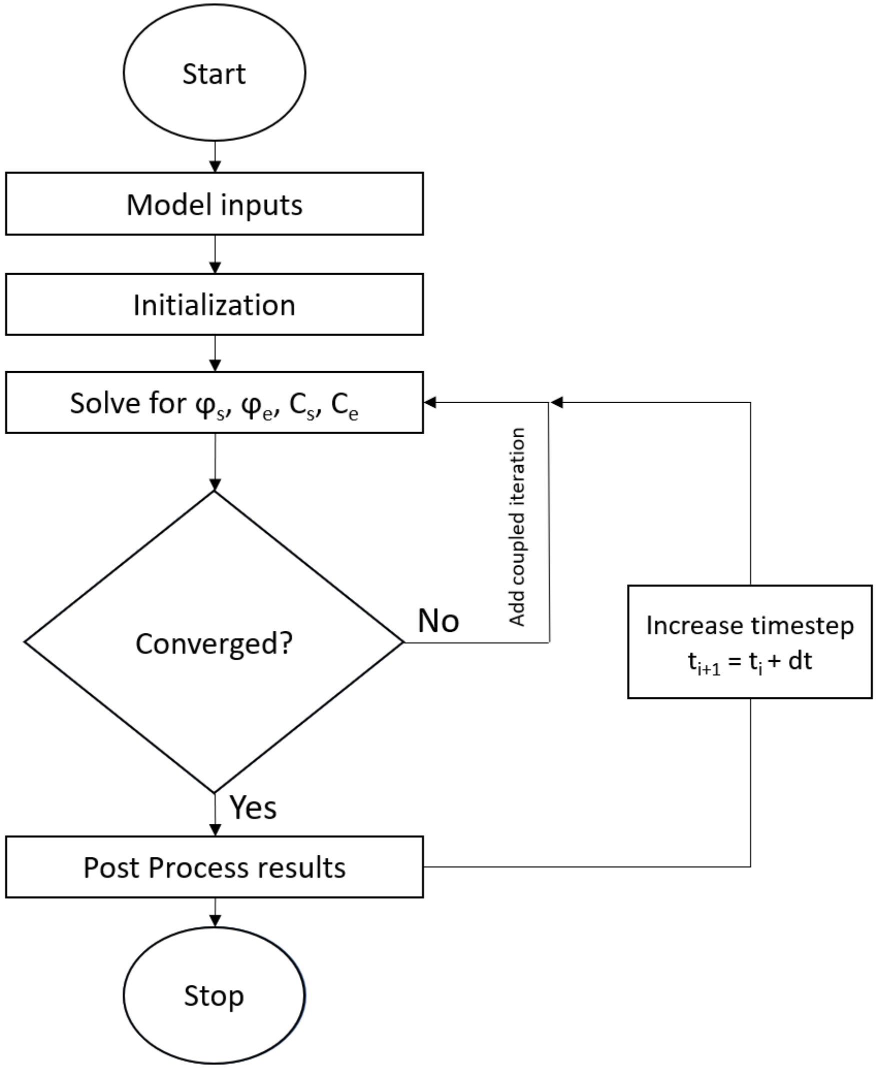


Figure: Timo Uimonen, Univ. Of Vaasa, 2020

Lithium-Ion battery- battery discharge

- Comparison show reasonable agreement with experimental results and other codes
- New model put under open source just few days ago
- See Ch. 69 of Elmer models manual
- Test case "**BatteryDischarge**"

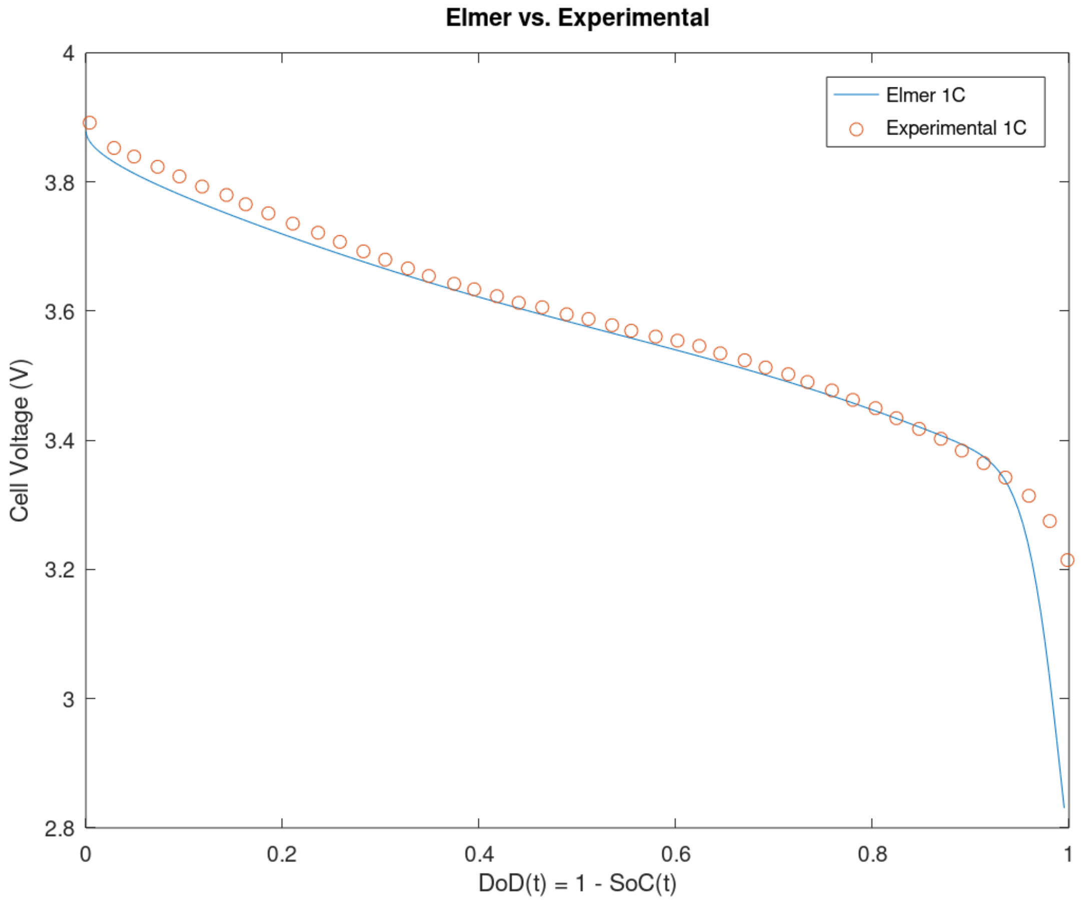
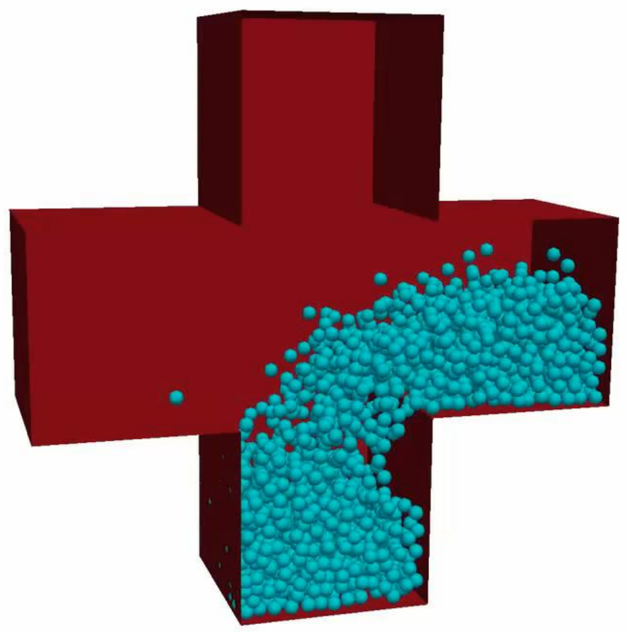


Figure: Timo Uimonen, Univ. Of Vaasa, 2020

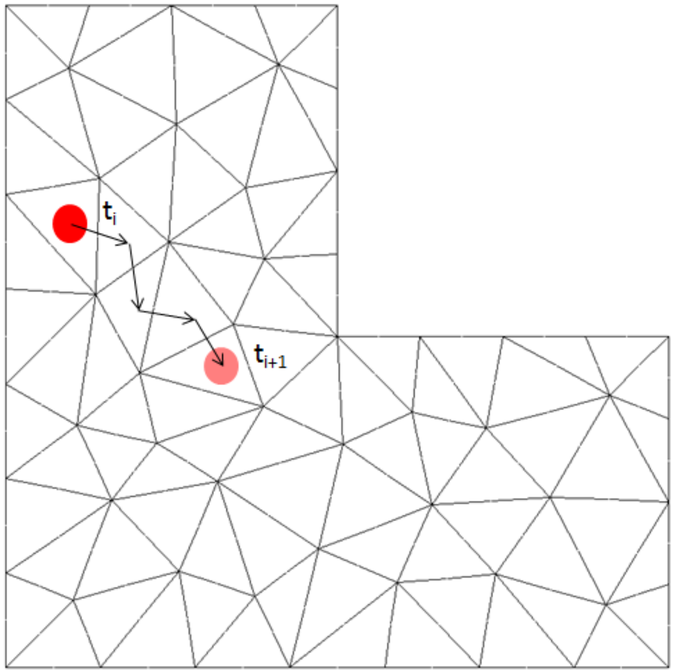
Coupling FEM and particle methods – heterogeneous models

- Finite element methods provide great way to model PDEs
    - Excel's for elliptic equations
    - Pure transport problems are challenging
    - Numerical diffusion difficult to avoid
- Particle based methods complements FEM often nicely
    - Equations written in the coordinate moving with the particle
- Back- and forth coupling with FEM!



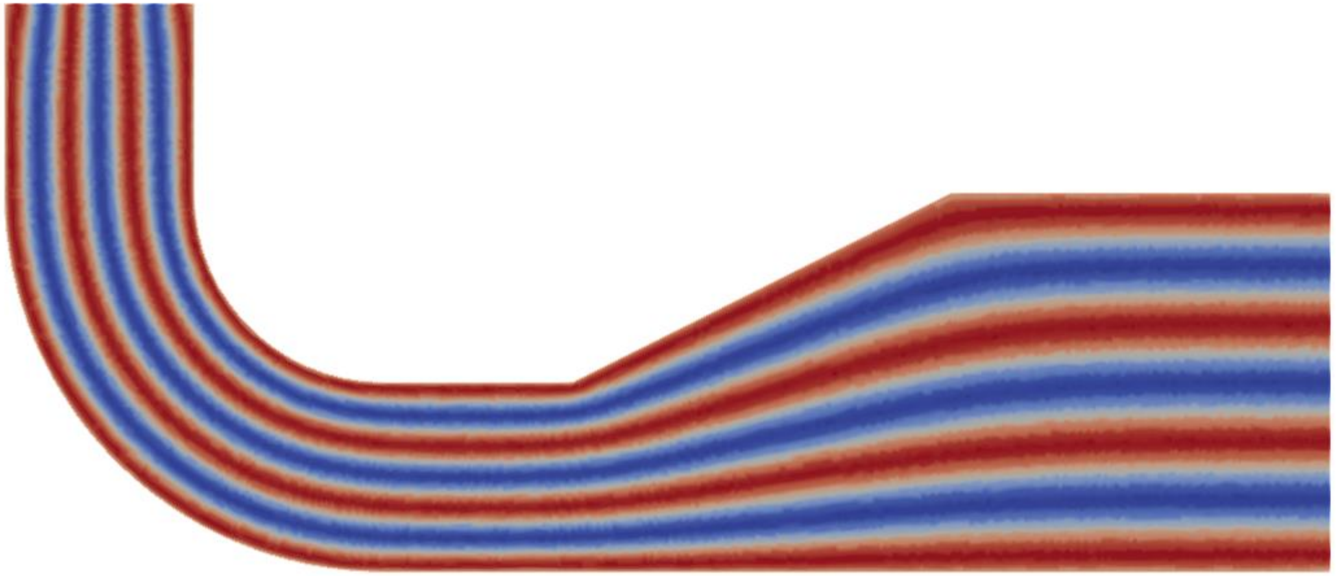
Particle tracking algorithm

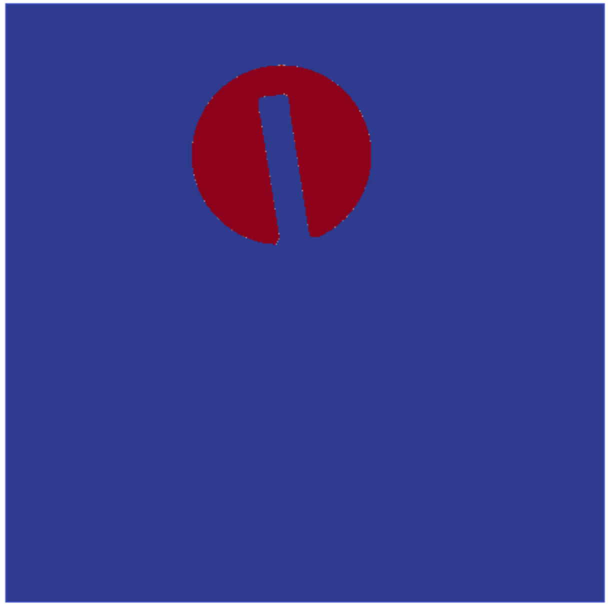
- Problem: Locate a particle in the finite element mesh
- Octree based search
  - Scales as N log(N)
  - Same cost for each step
  - Used in Elmer in mesh-to-mesh mapping
  - More difficult to parallelize effectively?
- **Marching search**
  - March from element-to-element
  - Initial price scales as N^(1/dim)
  - When the previous parent element is known the additional work is independent of mesh size
  - It is reasonable that the timestep is so small that the particle remains in the same element, or is in the neighbour element



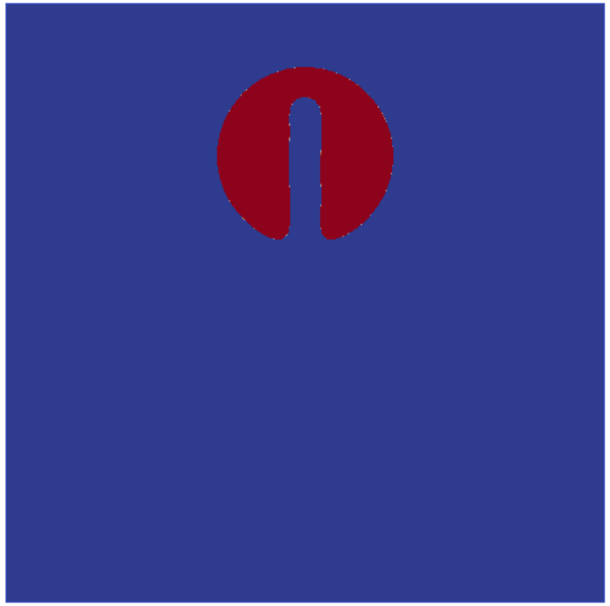
Hierarchical coupling to FEM: ParticleAdvector

- Hierarchical coupling to flow field
- Ideal method for fully convective problems
- Follow particles backward in time and register the field value
- Advected quantities: time & passive scalars
- We may compute advected fields at nodes, elements, and integration points



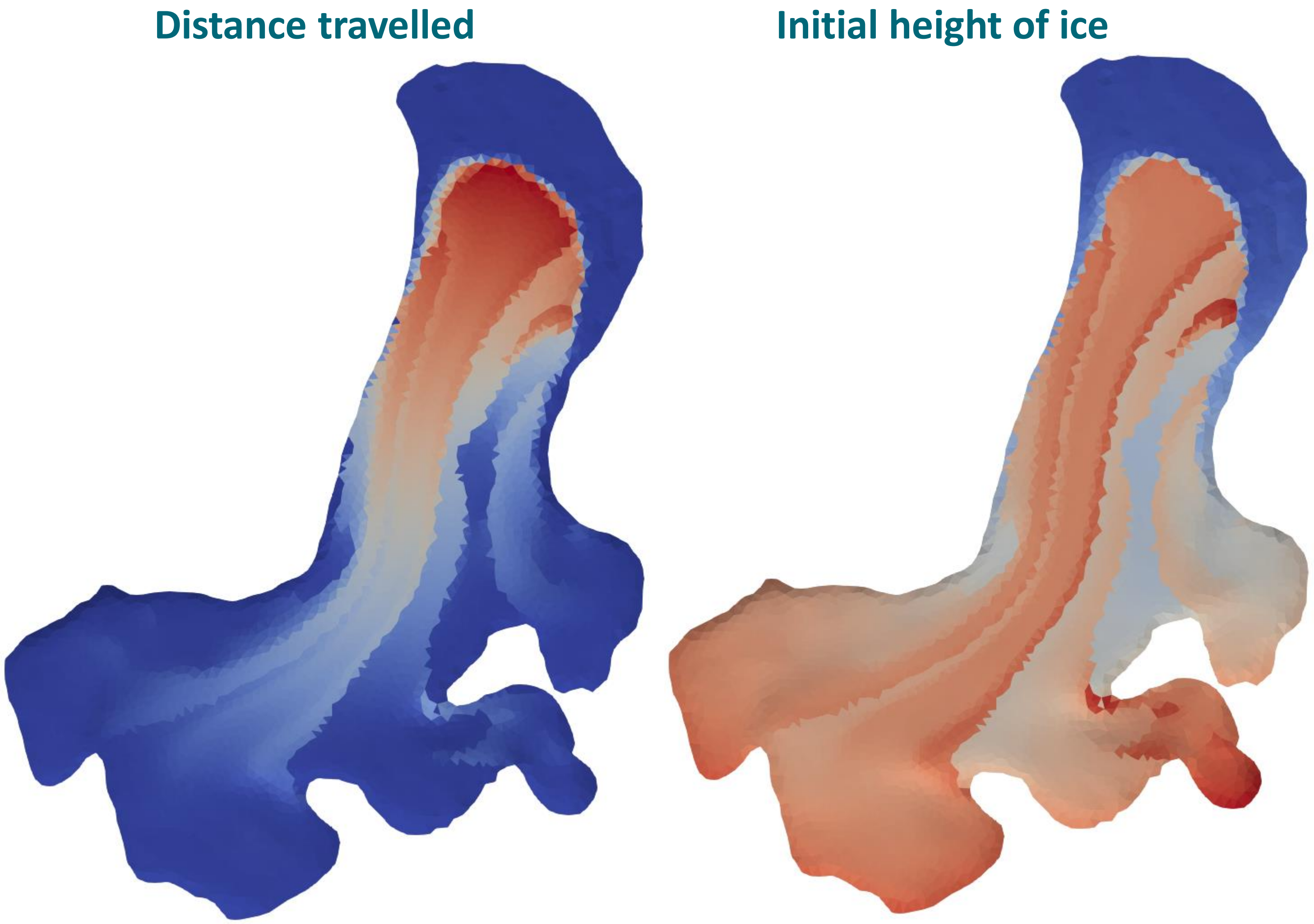


360°



ParticleAdvector – advection on glaciers

- Applied here to the Midtre Lovénbreen glacier
- Flow field of ice has been computed with Stokes equation
  - IncompressibleNSVec
- ParticleAdvector may be used to find the origin of the ice
  - Distance
  - Heigt
  - Age
  - etc.



Geometry from Välisuo, I., T. Zwinger and J. Kohler (2017), Journal of Glaciology, 1-10, doi:10.1017/jog.2017.26.

Bi-directional coupling to particles: ParticleDynamics

- Allow coupling between particles and fields
- Fields in the mesh affect particles
    - Particle knows its position in the mesh
    - Particle may be influenced by the fields in the element at its exact location
    - Forces due to: electrostatic & magnetic field, viscous drag, etc.
- Particles contribute to material properties or source terms of the PDEs
    - Carriers of property (several type of particles)
    - Particles may be sources of electric charge, heat etc.
    - Contribution is shared among the nodes of the element

FEM-particle coupling: Self-consistant Poisson equation

FEM: $$-\nabla \cdot \varepsilon \nabla \phi = \rho + \sum_i q_i \, \delta(\vec{r} - \vec{r_i})$$

$$\sum_i q_i \, \delta(\vec{r} - \vec{r_i})$$

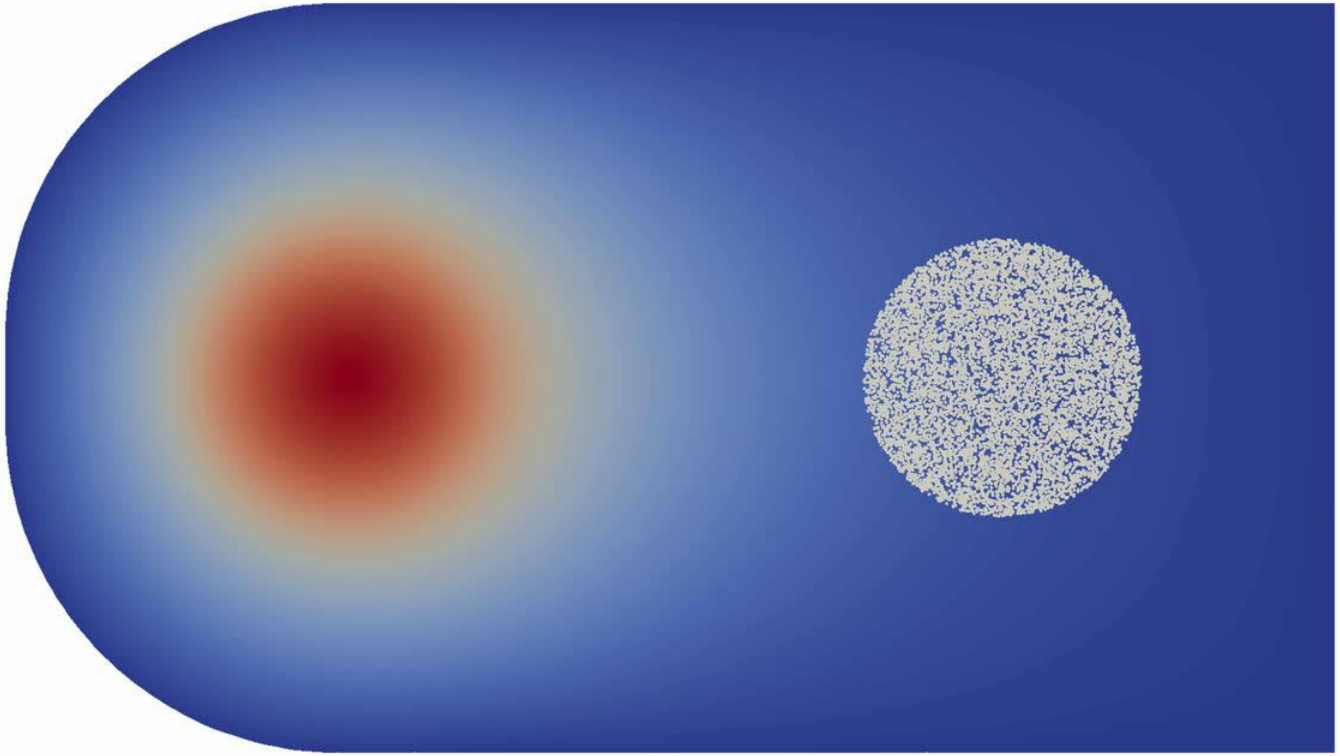
$$\nabla \phi(\vec{r}) \approx \sum_{j=1}^{n} \phi_j \nabla \psi_j(\vec{r})$$

MC:
$$\vec{v}^{(i+1)} = \vec{v}^{(i)} + \frac{dt}{m} \sum_j \vec{f}^j ,$$
$$\vec{r}^{(i+1)} = \vec{r}^{(i)} + dt \, \vec{v}^{(i+1)} .$$

MMM @HPC

- EU project aiming for multiscale modeling of materials
- Our goal was to solve self consistent Poisson equation with free particles
  - Poisson equation solved with FEM
  - Particles tracked using Newton's equations

FEM-particle coupling – self consistant Poisson



A toy case where free charged particles move to cancel out the potential of the fixed charge. Simulation Peter Råback, CSC.

FEM-particle coupling: Tectonic flow

- Particles carry the initial material properties
- We can compute fraction of particle types from the particle trace
- Used to model viscosity and density
- Test case: **ParticleFallingBlock** (related to tectonic flows)

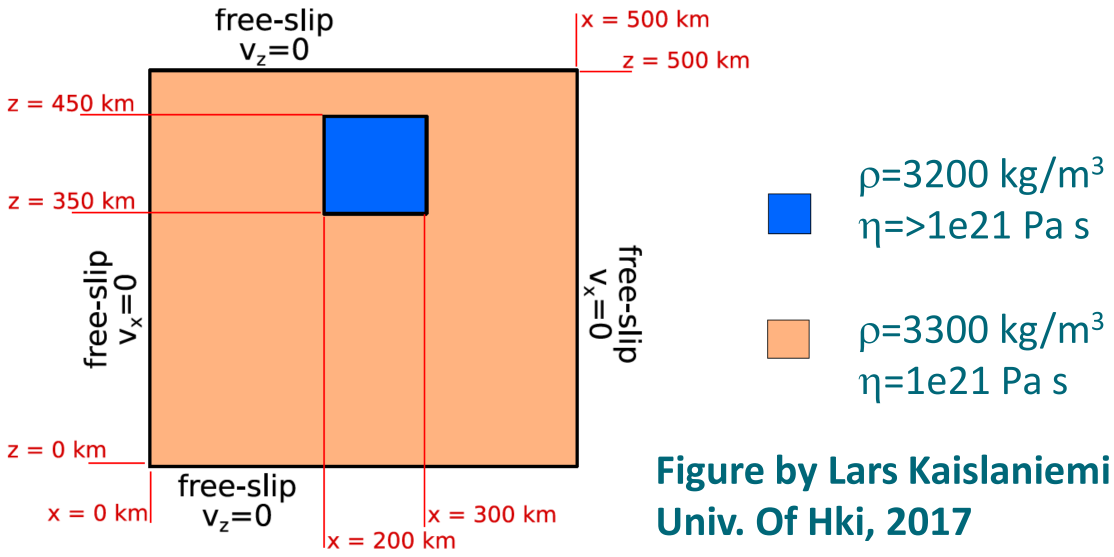
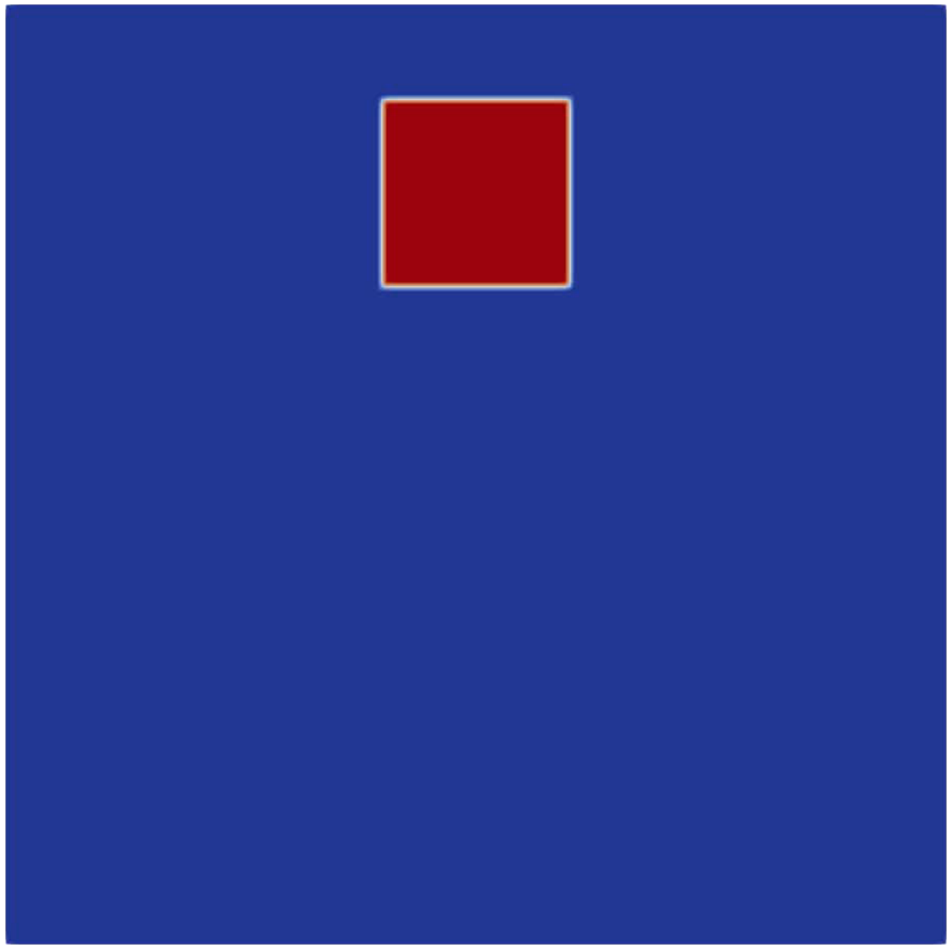
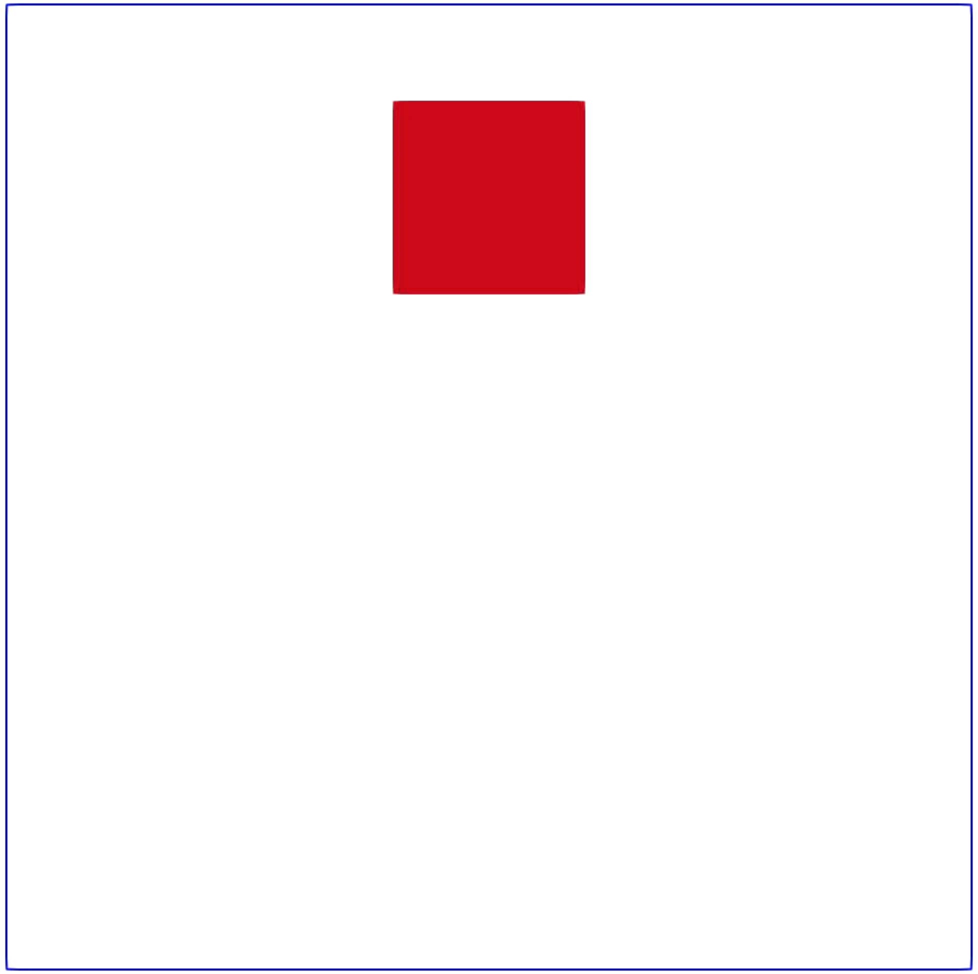


Figure by Lars Kaislaniemi
Univ. Of Hki, 2017



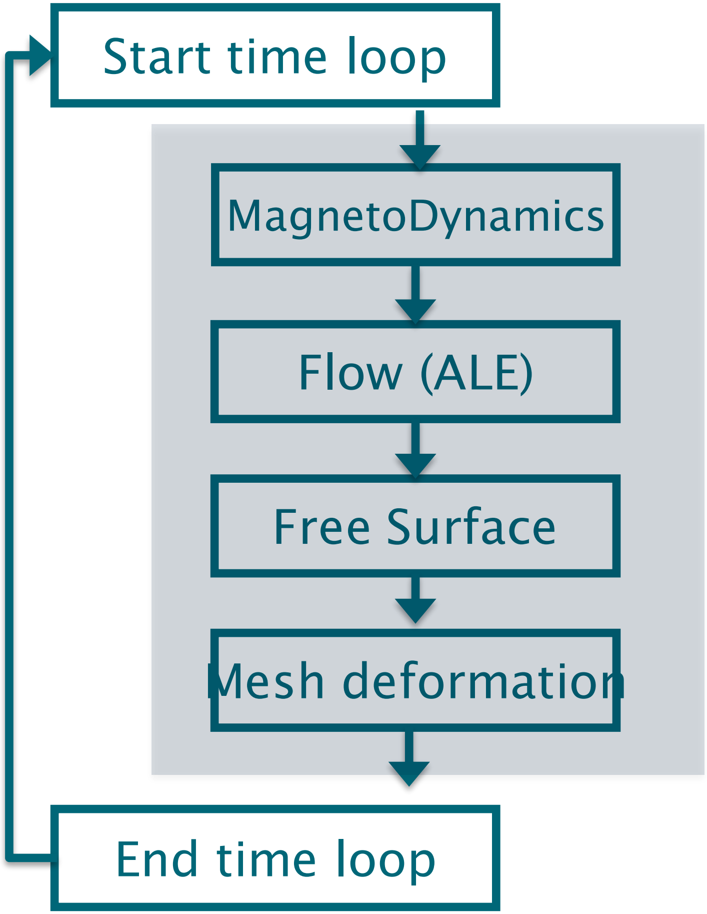
FEM-particle coupling: the bad

- For many uses the number of particles should be very large
  - Much larger than typical number of Gaussian integration points
- For such cases the machinery of Elmer is rather slow
  - Usually efficient particle-based methods follow particles in a uniform background mesh
- For serious uses dedicated codes such as LAMMPS are preferrable
- Tracer particles and ParticleAdvector ok!



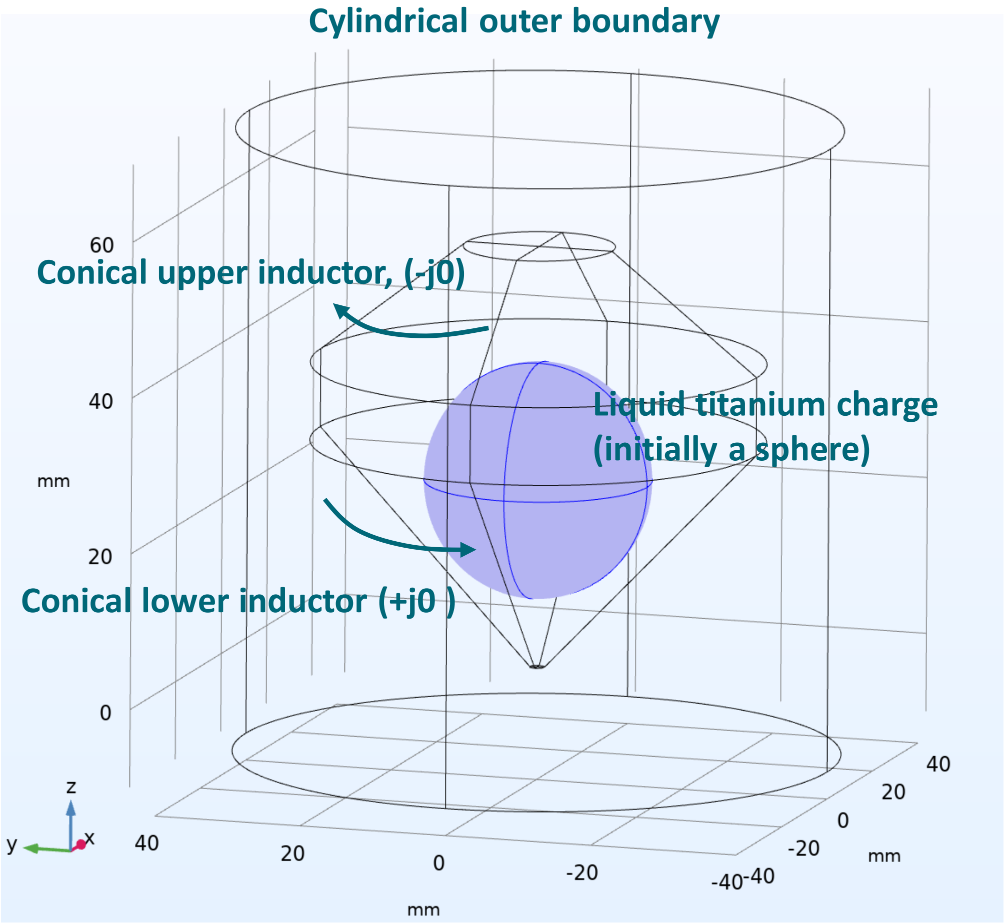
Magnetic levitation – loose coupling in magnetohydrodynamics

- One of the strengths of Elmer is modeling of magnetic fields
- Could this be coupled with Navier-Stokes equation with free surface?
  - Lagrangian solution with mesh velocity defined (ALE formulation)
- Mesh deformation needed to update the mesh to the deformed shape
- Iterative coupling
  - Only conditionally stable



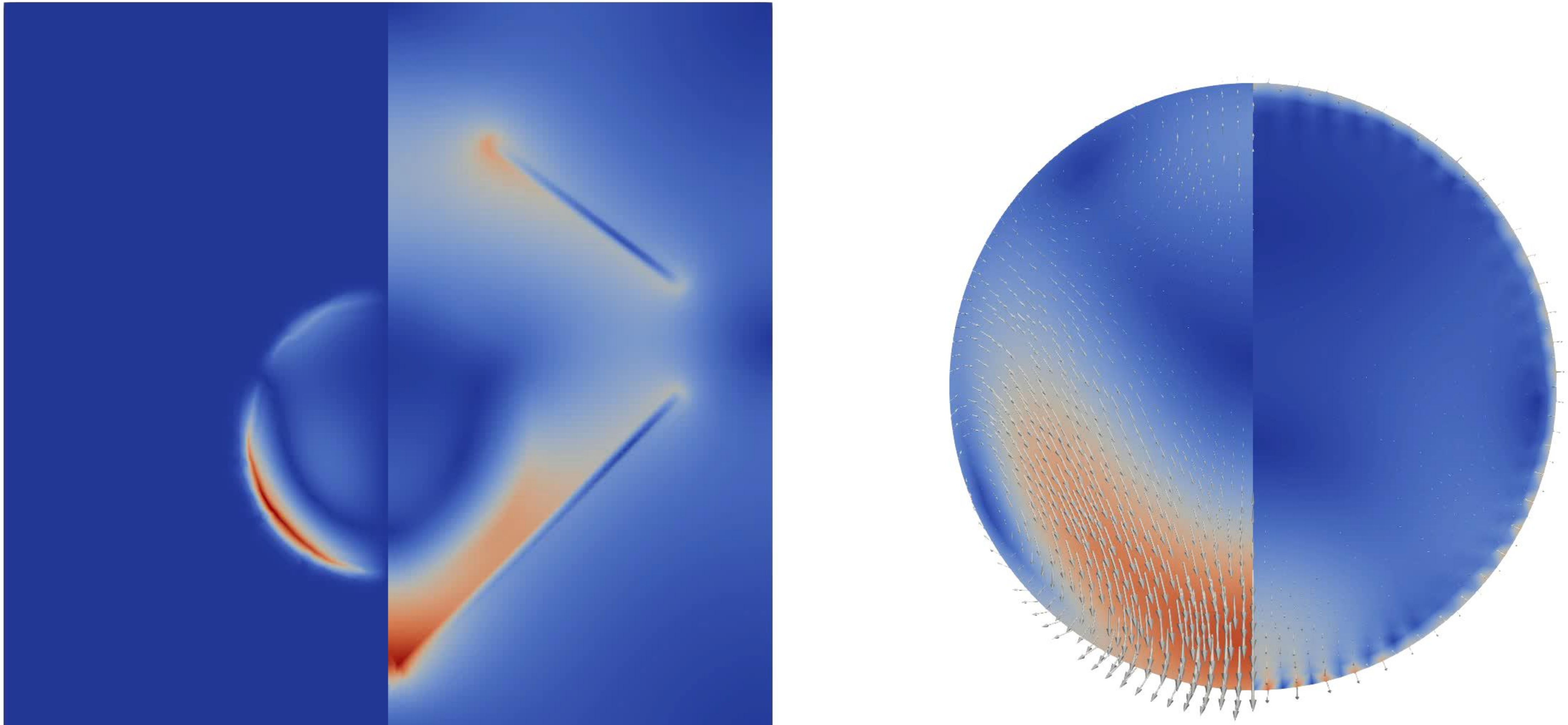
EM levitation model – rotationally symmetric test case

- Test case suggested by Roland Ernst
  - See Elmer discussion forum under "**EM Levitation**"
- In principle Elmer has all the features needed
- The initial transients where not easily captured (conditional stability)
  - Resulted to small timesteps
- Parameter space is challenging
  - Preliminary results for easier parameters



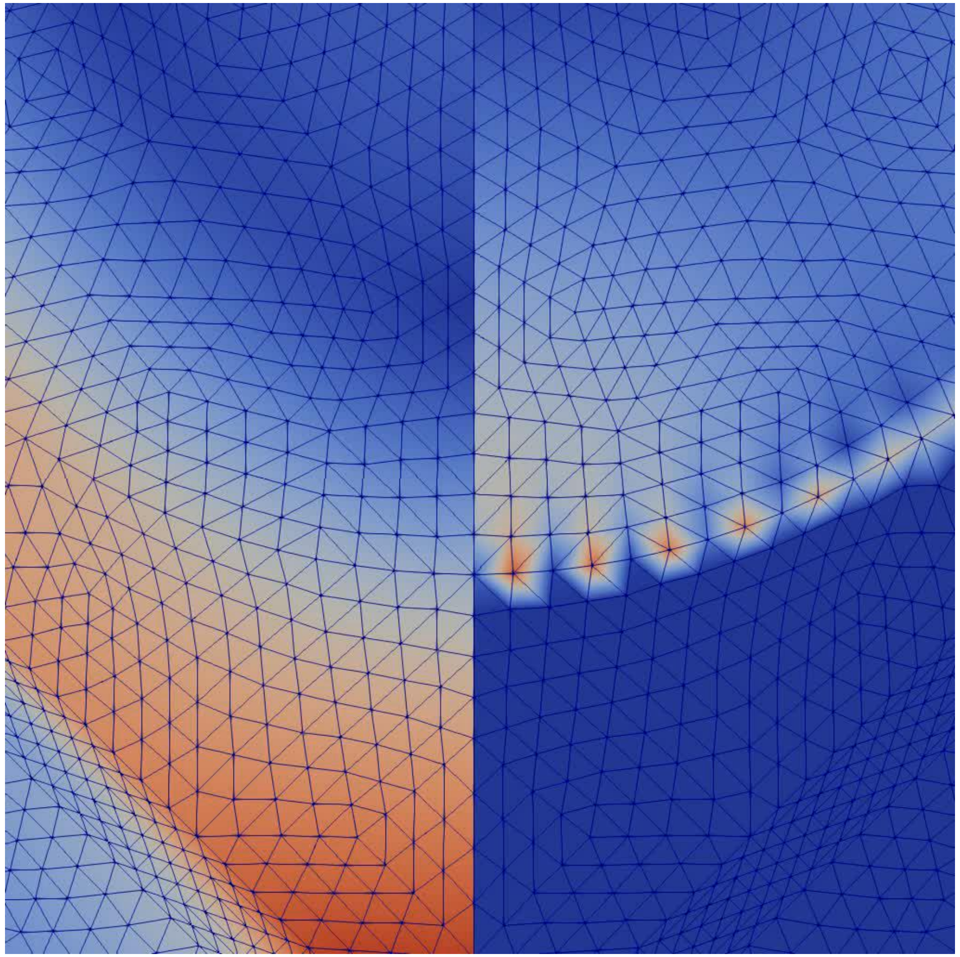
Test case specification by Roland Ernst, 2021

EM levitation model – preliminary results



EM levitation - need for robust Eulerian strategy

- When the liquid becomes distorted there is no easy remedy with Lagrangian methods
- Elmer does not have too robust Eulerian methods for free surfaces
- There exists an optiomal solution for this kind of problem combining two software
  - In multiphysics one software may not always be enough...
- EOF Library combines OpenFOAM and Elmer is a efficient way on MPI level!
  - https://eof-library.org/



Comparison of loose and tight coupling

Loose (segregated)

- May not converge for strongly coupled problems
- Easy to utilize existing solvers for individual problems
- No need to estimate cross terms of Jacobian
- Simple matrix equations more easily solved by optimal (multigrid) methods
- Efficient memory use

Tight (monolithic)

- Robust method for coupled problems in the whole parameter space
- Reuse of existing solvers more difficult
- Cross terms of Jacobian may be difficult to estimate
- Resulting monolithic matrix may be ill-conditioned limiting choice of linear solvers
- Often real memory hogs

Combining the merits of tight and loose coupling

- Is it possible to construct methods that combine some of the good features of loose and tights coupling?
  - **Robust** convergence for the coupled problem in the whole parameter space
  - Use of **optimal linear solvers** for individual subproblems
  - **Reuse** of individual solvers
  - Efficient **memory** use
  - …
- Yes, different strategies may eliviate different problems
  - Strategies on the continuous level - physically motivated
    - e.g. artificial compressiblity in FSI
  - Strategies on the discrete level - numerically motivated
    - e.g. block preconditioning

Most important Elmer resources

- http://www.csc.fi/elmer
  - Official Homepage of Elmer
- http://www.elmerfem.org
  - Discussion forum, wiki, elmerice community
- https://github.com/elmercsc/elmerfem
  - GIT version control (the future)
- http://youtube.com/elmerfem
  - Youtube channel for Elmer animations & webinars
- http://www.nic.funet.fi/pub/sci/physics/elmer/
  - Download repository
- Further information: peter.raback@csc.fi

Thank you for your attention!