Geophysical applications beyond
(but in connection to)
Elmer/Ice

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Elmer FEM webinar
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With contributions by

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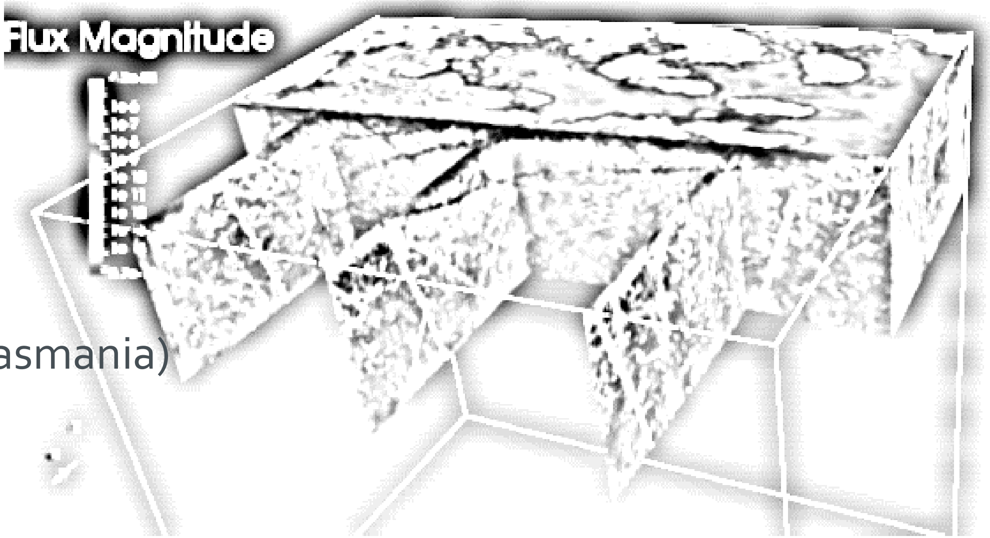
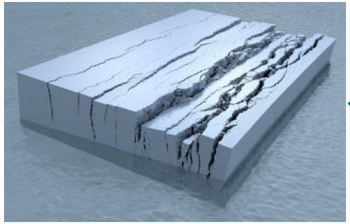
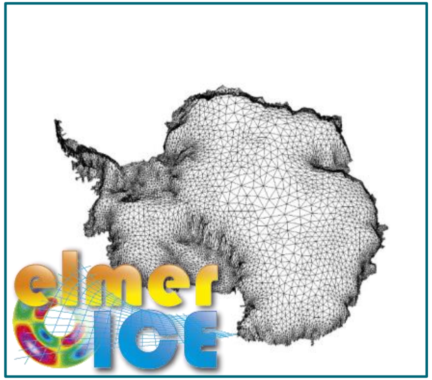
- **Matt King** (Univ. Tasmania)
- **Grace Nield** (Univ. Durham + Univ. Tasmania)



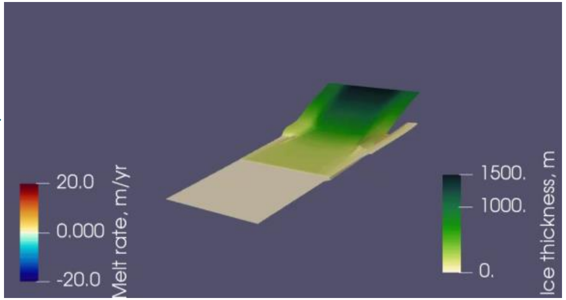
Beyond Elmer/Ice

Coupler to DEM (HiDEM)

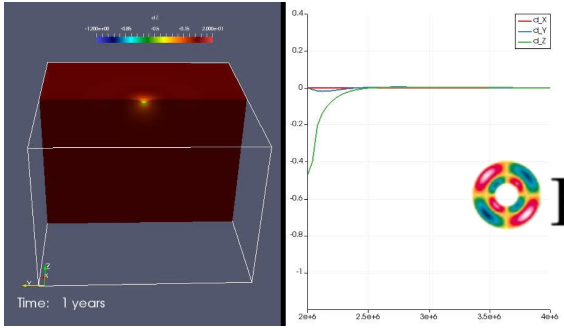




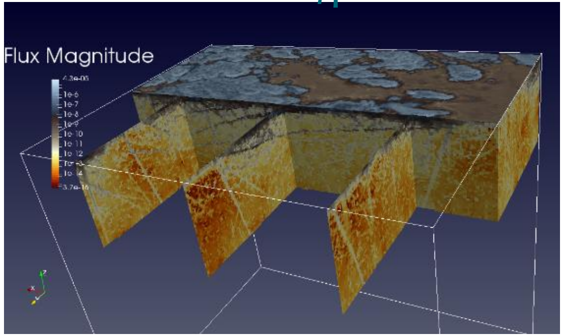
Ice-ocean coupler (FISOC)



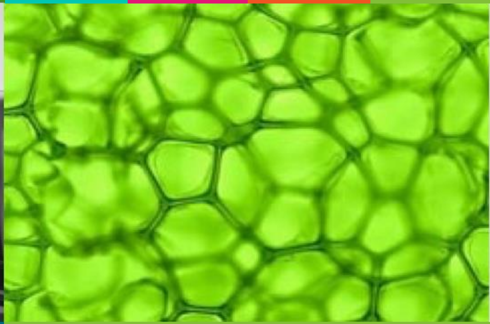
Visco-elastic earth model



Groundwater/permafrost model

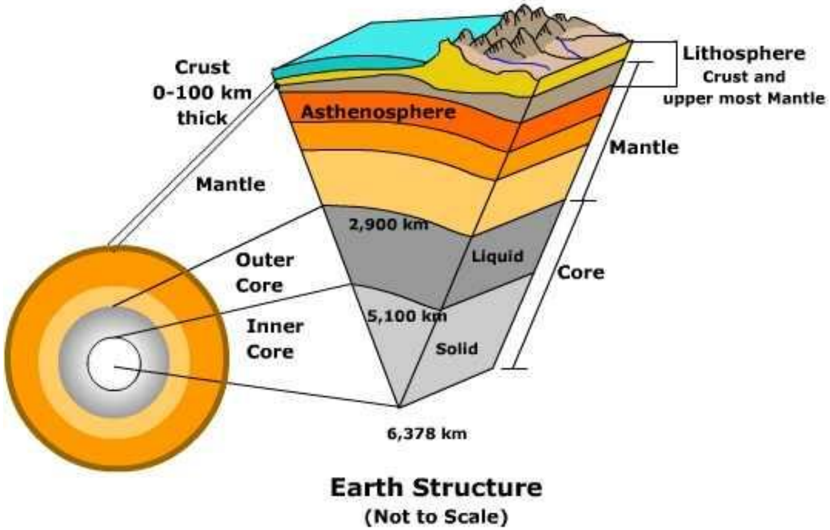


Viscoelastic earth model



Structure of Earth

- Lithosphere:
  - Earth's crust only in average 20 km thick (~ brittle, elastic plate)
    - Minerals; $\rho \approx 2900 \text{ kg m}^{-1}$
  - Asthenosphere (mineral upper part of mantle):
    - $c; \eta \approx 10^{19} \ldots 10^{21} \text{Pa s}$
- Mantle:
  - All in all 2900 km thick; mineral
  - At bottom $\rho \approx 5700 \text{ kg m}^{-1}$
- Core (metallic):
  - $\rho \approx 9400 \longmapsto 13500 \text{ kg m}^{-1}$
  - Outer, 3200 km thick liquid core
  - Inner, 1200 km thick solid core



Picture taken from http://www.sfu.ca/geog/geog351fall06/group06/Image/Earthquake/EQ%20Pictures/earth_structure.jpg

Structure of Earth

- Earth has a layer type of structure
- Determined by seismic measurements
- PREM (Preliminary

Physics of the Earth and Planetary Interiors, 25 (1981) 297–356
Elsevier Scientific Publishing Company, Amsterdam – Printed in The Netherlands

Preliminary reference Earth model *

Adam M. Dziewonski [1] and Don L. Anderson [2]

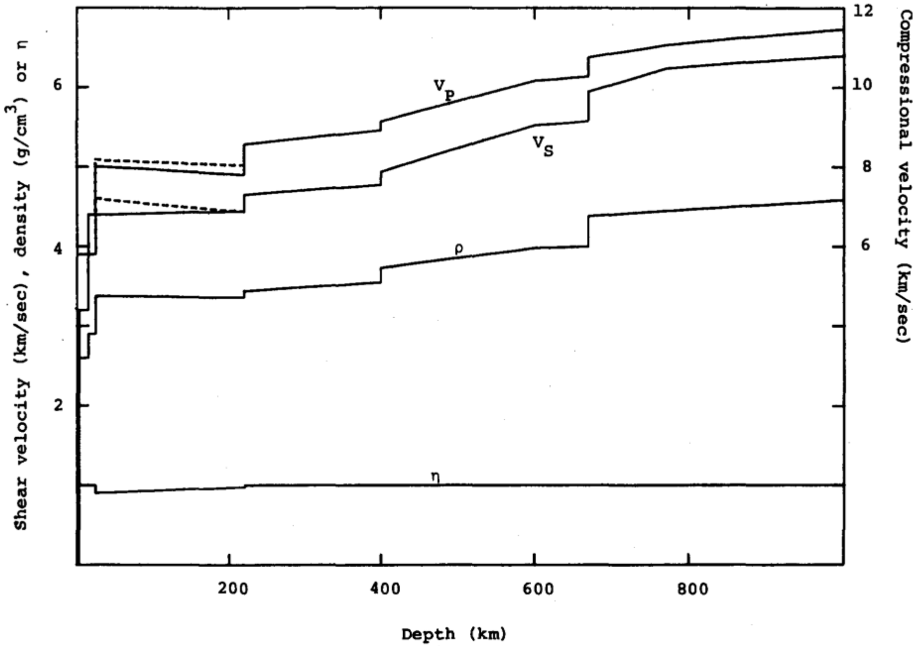
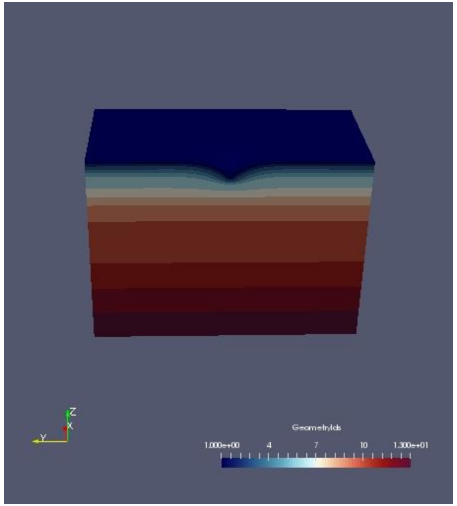


Fig. 7. Upper mantle velocities, density and anisotropic parameter η in PREM. The dashed lines are the horizontal components of velocity. The solid curves are η, ρ and the vertical, or radial, components of velocity.

Structure of Earth

Layer	Layer top (radius, km)	Layer base (radius, km)	Thickness (km)	Viscosity	Density	Young's Modulus	Poisson's Ratio	Gravitational Acceleration
Lithosphere	6371	6336	35	1x10^44	3196	1.8148E+11	0.4	9.7852
Lithosphere	6336	6301	35	1x10^44	3196	1.8148E+11	0.4	9.7852
Lithosphere	6301	6251	50	1x10^44	3196	1.8148E+11	0.4	9.7852
Upper Mantle	6251	6201	50	1x10^18	3439	2.1901E+11	0.4	9.8367
Upper Mantle	6201	6141	60	1x10^18	3439	2.1901E+11	0.4	9.8367
Upper Mantle	6141	5971	170	1x10^18	3439	2.1901E+11	0.4	9.8367
Upper Mantle	5971	5835	136	1x10^18	3882	3.2393E+11	0.4	9.9349
Upper Mantle	5835	5701	134	1x10^18	3882	3.2393E+11	0.4	9.9349
Lower Mantle	5701	5450	251	1x10^22	4527	5.3663E+11	0.4	9.9799
Lower Mantle	5450	4770	680	1x10^22	4527	5.3663E+11	0.4	9.9799
Lower Mantle	4770	4340	430	1x10^22	5074	7.2010E+11	0.4	9.9108
Lower Mantle	4340	3910	430	1x10^22	5074	7.2010E+11	0.4	9.9108
Lower Mantle	3910	3480	430	1x10^22	5074	7.2010E+11	0.4	9.9108

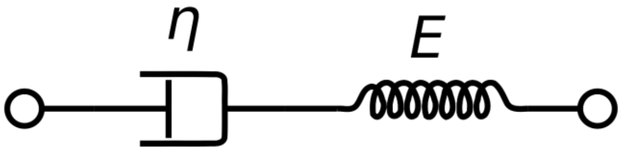


Non-self gravitating *Flat-earth model*

Implementation in Elmer

- Standard FE *linear elasticity*: $\nabla \cdot \boldsymbol{\tau} = \mathbf{0}$
- Elastic rheology: stress as a function of reversible deformation
- Visco-elastic – Maxwell rheology :

(partly non-reversible) deformation as a function of



viscous and elastic contribution

Implementation in Elmer

- Introduction of visco-elastic stress (Wu 2004)

$$\frac{\partial \boldsymbol{\tau}}{\partial t} = \frac{\partial \boldsymbol{\tau}_0}{\partial t} + \frac{\mu}{\eta}(\boldsymbol{\tau} - \Pi \mathbf{1})$$

$$\boldsymbol{\tau}_0 = \Pi \mathbf{1} + 2\mu\boldsymbol{\epsilon}$$

(Maxwell time)$^{-1}$

  - At the same time we introduce pressure Π to enable incompressibility

- Additional term accounting for restoring force by specific weight gradient (aka. pre-stress advection)

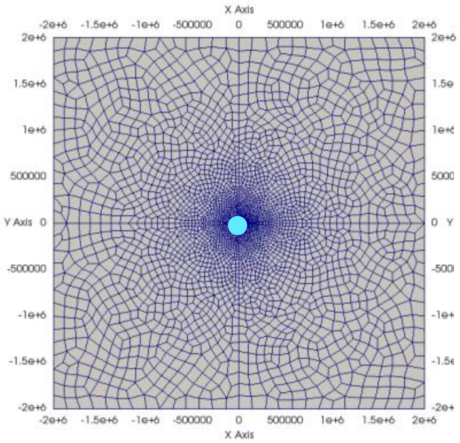
$$\nabla \cdot \boldsymbol{\tau} - \rho g \nabla(\boldsymbol{e}_z \cdot \boldsymbol{d}) = \mathbf{0}$$

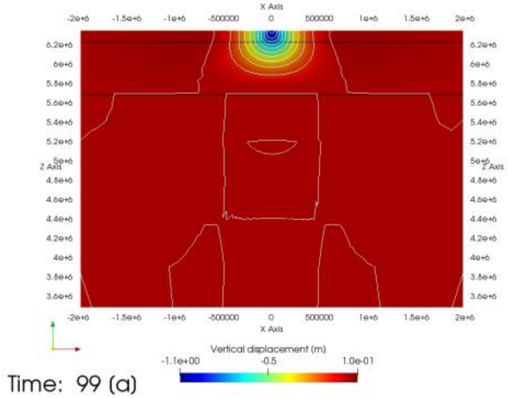
  - This is not standard in commercial FE packages, hence needs to be "cheated" around by putting jump-conditions on inter-layer boundaries (Winkler foundations)
  - In Elmer we can include this, which introduces the right boundary condition naturally from the third term of the weak formulation

$$\int_\Omega \tau(\boldsymbol{u}) \cdot \boldsymbol{\epsilon}(\boldsymbol{v})\, dV - \oint_{\partial\Omega} (\tau(\boldsymbol{u}) \cdot \boldsymbol{n}) \cdot \boldsymbol{v}\, dA - \int_\Omega \rho g \nabla(\boldsymbol{e}_z \cdot \boldsymbol{u}) \cdot \boldsymbol{v}\, dV = 0.$$

GIA benchmark model

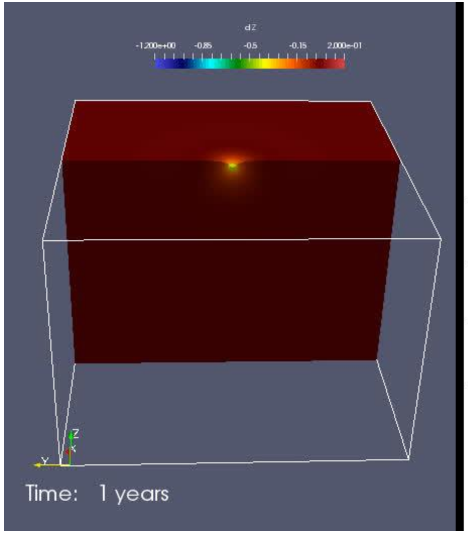
- Total width 4000km (2000km each side of the ice load centre)
- Depth – surface to core (6371 – 3480km)
- Load:
  - Disc radius: 50km (diametre 100km)
  - Disc thickness: 100m
  - Ice density: 917 kg/m3
  - Loading 100 years, unloading 100 years

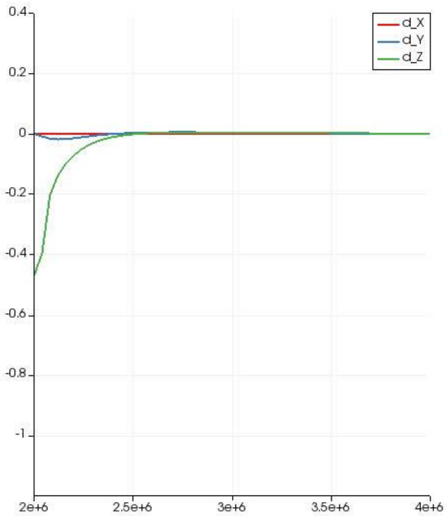




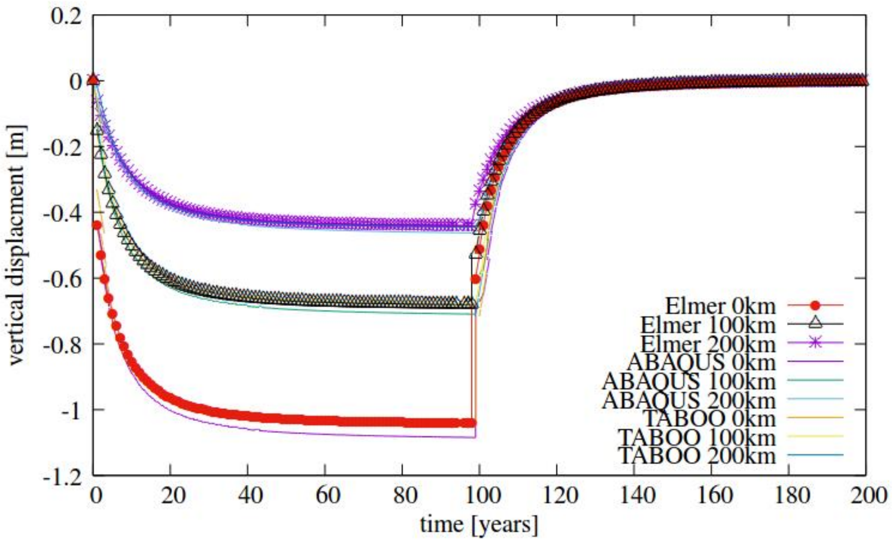
Zwinger, T., Nield, G. A., Ruokolainen, J., and King, M. A., 2020. ***A new open-source viscoelastic solid earth deformation module implemented in Elmer (v8.4)***, Geosci. Model Dev., **14**, 1155–1164, doi:10.5194/gmd-13-1155-2020

GIA benchmark model





GIA benchmark model – comparison to ABAQUS and TABOO

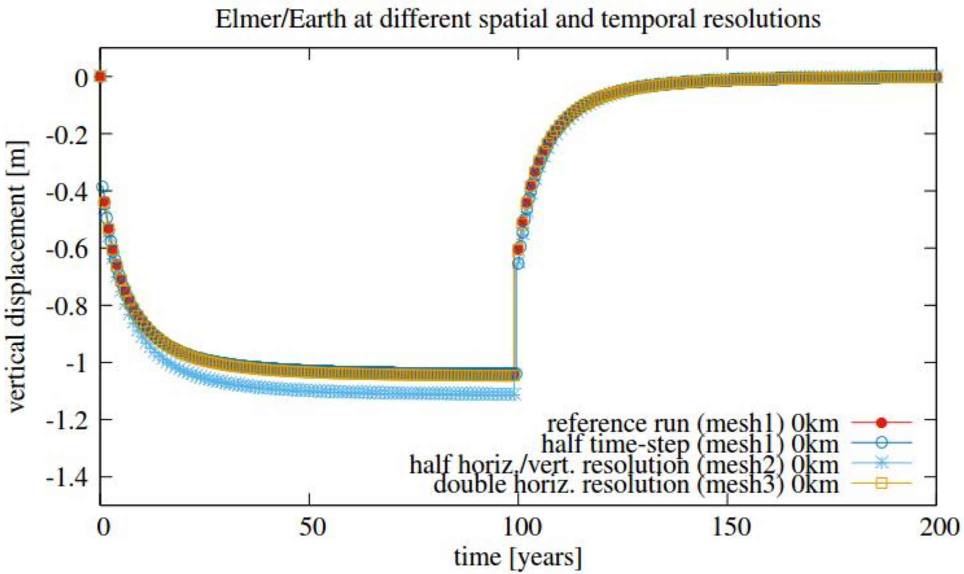


- ABAQUS: FEM model run at constant 25 km horizontal resolution
- TABOO: post-glacial rebound calculator (Spada et al., 2003) using classical visco-elastic normal mode method.
    - Incompressible, non-rotating, self-gravitational
    - Spherical harmonics degree 2048 (equivalent to approximately 10km)

GIA benchmark model – accuracy and performance

name	elements	min hor. res.
mesh 1	80k	~10 km
mesh 2 (half)	40k	~25 km
mesh 3 (double)	150k	~5 km

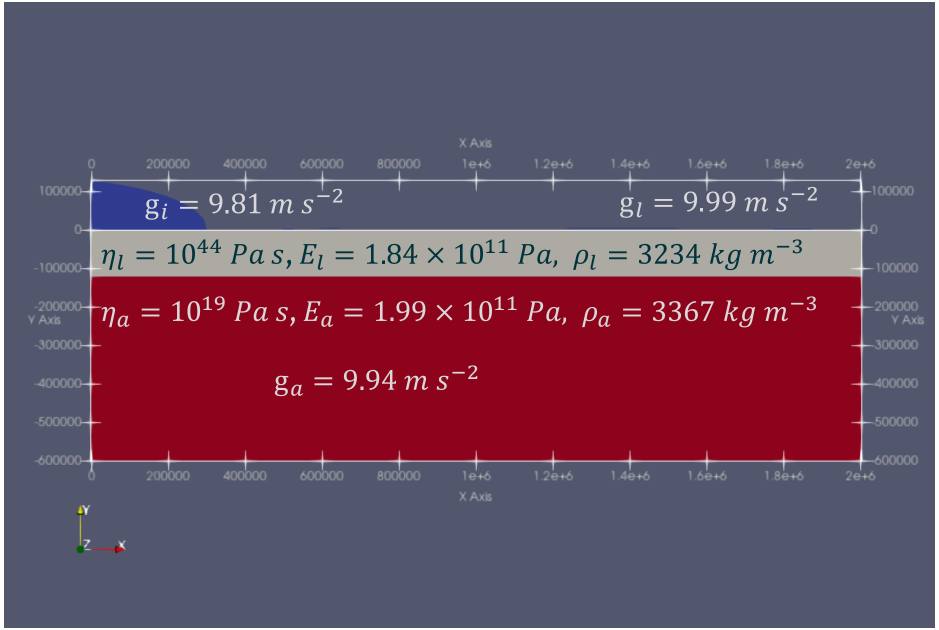
name	partitions	time [s]
mesh 1	16	21 200
mesh 1 (strong)	32	9600 (2.2 speedup)
mesh 3 (weak)	64	15800 (0.61 scaled speedup)



Simple 2D/2layer testcase in source code:
`elmerfem/fem/tests/elmer_earth_2d_2layer/`

Coupled to ice sheet

- Imposing ice sheet with a Bueler profile
- 5 kyr advance from 0-300km (1500 m thickness)
- 5 kyr retreat
- 2 layer model (crust 12 km + mantle 600 km)



Coupled to ice sheet

```
!=============================================================
!---------------- MATERIALS ----------------------
!=============================================================
Material 1
  Name = "Ice Material"
  Density = Real #rhoi
End
! Lithosphere
Material 2
  Density =  #rhol
  Damping = Real 0.0
  Youngs Modulus = #ymodl
  ! supper high viscosity, hence,
  ! Maxwell time is such that it acts elastic
  Viscosity = #viscl
  Poisson Ratio = Real 0.49 !not needed if incompressible
End
! Upper Mantle 1
Material 3
  Density =  #rhoa
  Damping = Real 0.0
  Youngs Modulus = #ymoda
  Viscosity =#visca
  Poisson Ratio = Real 0.49 !not needed if incompressible
End
```

$$\frac{\partial \boldsymbol{\tau}}{\partial t} = \frac{\partial \boldsymbol{\tau}_0}{\partial t} + \frac{\mu}{\eta}(\boldsymbol{\tau} - \Pi \mathbf{1})$$

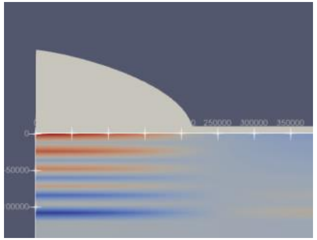
```
!=============================================================
!---------------- BODY FORCES ----------------------
!=============================================================
Body Force 1
  Name = "Ice Bodyforce"
  Flow BodyForce 1 = Real 0
  Flow BodyForce 2 = Real #-gravity
End
! Lithosphere
Body Force 2
 Stress BodyForce 1 =  0.0
 Stress BodyForce 2 =  0.0
 Gravitational Prestress Advection = Logical True
 GPA Coeff = Real # rhol * gravl
End
!Upper Mantle 1
Body Force 3
 Stress BodyForce 1 =  0.0
 Stress BodyForce 2 =  0.0
 Gravitational Prestress Advection = Logical True
 GPA Coeff = Real # rhoa * grava
End
```

$$-\rho g \nabla(e_z \cdot \boldsymbol{d})$$

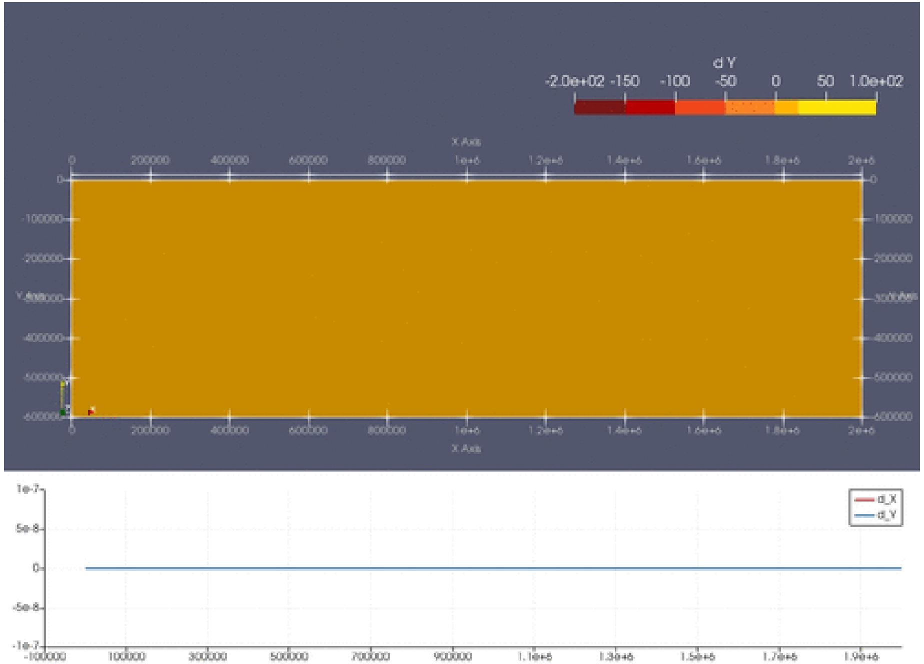
Coupled to ice sheet

```
!==============================================================================
! /// Visco-elastic solver ///
!==============================================================================
Solver 4
  Equation = "Elasticity Analysis"
  Procedure = "StressSolve" "StressSolver"

  Displace Mesh = Logical True ! physically deform the mesh?

  Calculate Stresses = Logical True ! outputs elastic stresses

  ! 2D: 2 deformation 1 pressure (as incompressible)
  Variable = String "t[d:2 p:1]"

  ! if using p:1 and bubble, then either b:3 or b:6
  !  Element = "p:1 b:3 "
  ! best to use p:2 for deofrmation (pressure will be p:1)
  Element = "p:2"

  ! Visco-elastic computation if Ture
  Maxwell material = Logical True
  Incompressible = Logical True
  Time Derivative Order = 1

  ! Numerical settings (here direct Solver)
  Linear System Solver = Direct
  Linear System Direct Method = MUMPS
  Steady State Convergence Tolerance= 1.0e-5
End
```

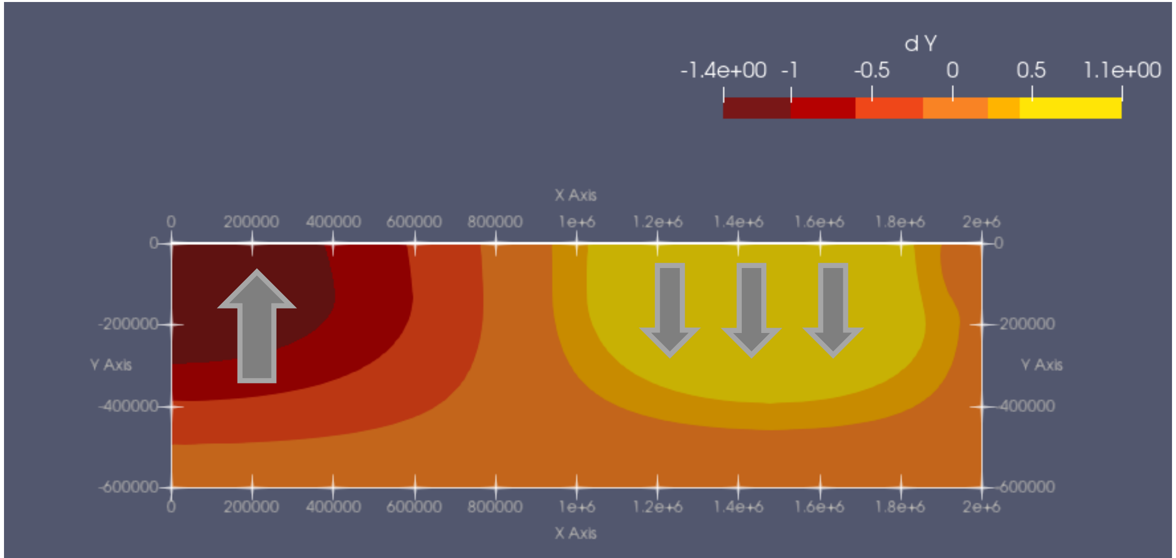
- Add-on functionality to existing linear elasticity solver (`StressSolve`)
- Incompressibility expects deformations + pressure DOF
- Best strategy for stabilization: p:2 (p:1)



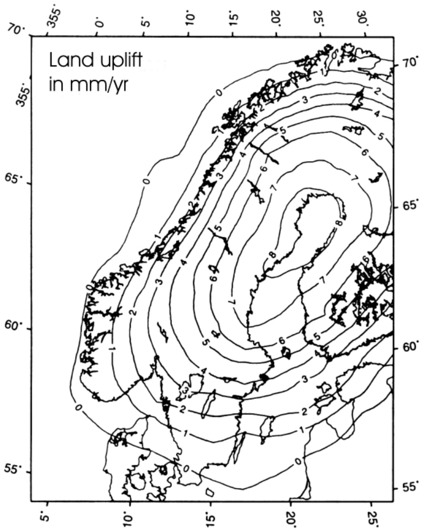
Coupled to ice sheet



Coupled to ice sheet

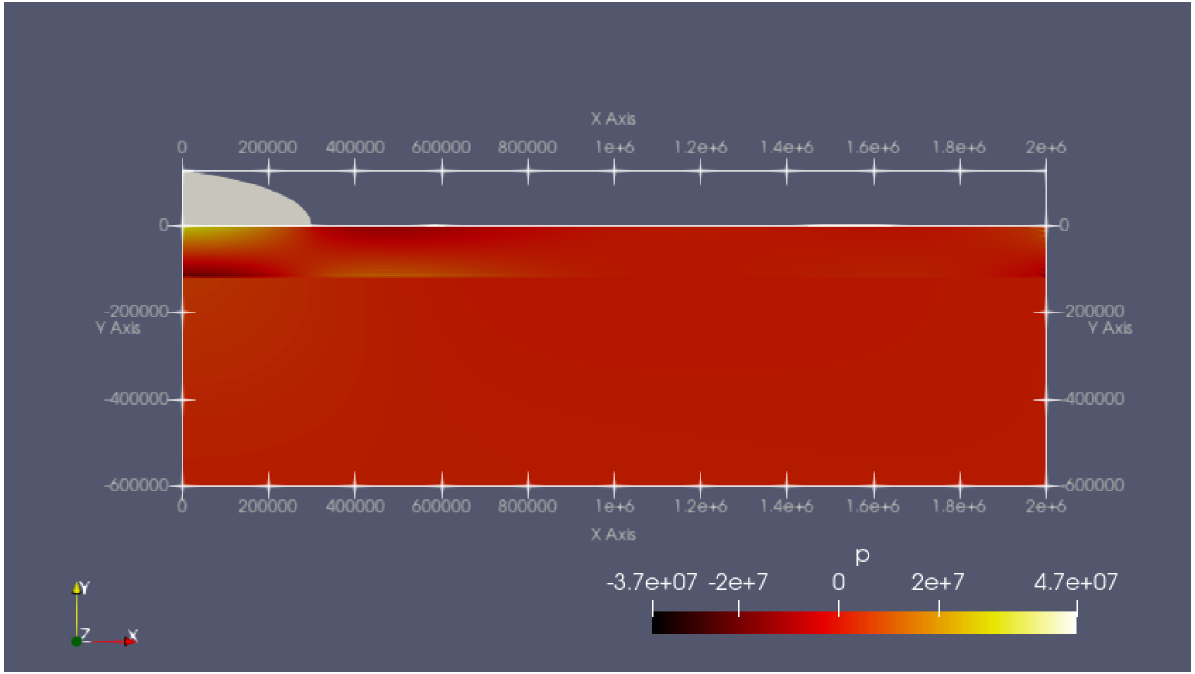


Remaining deformation after deglaciation

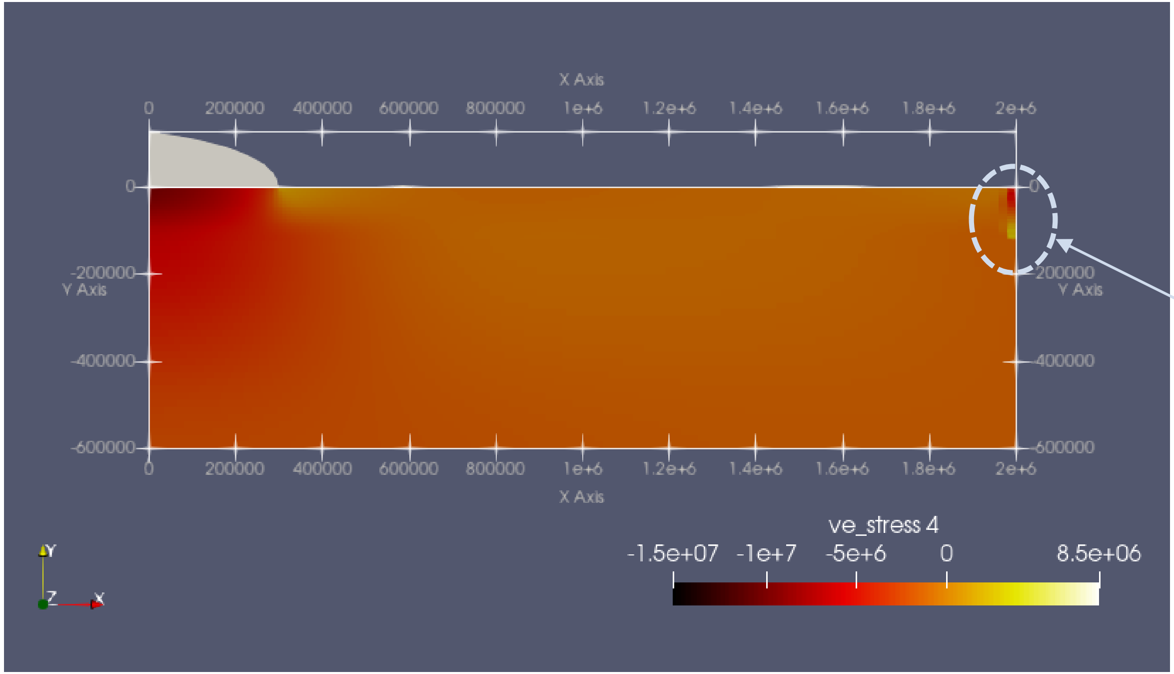


From Thoma and Wolf, 1999

Coupled to ice sheet

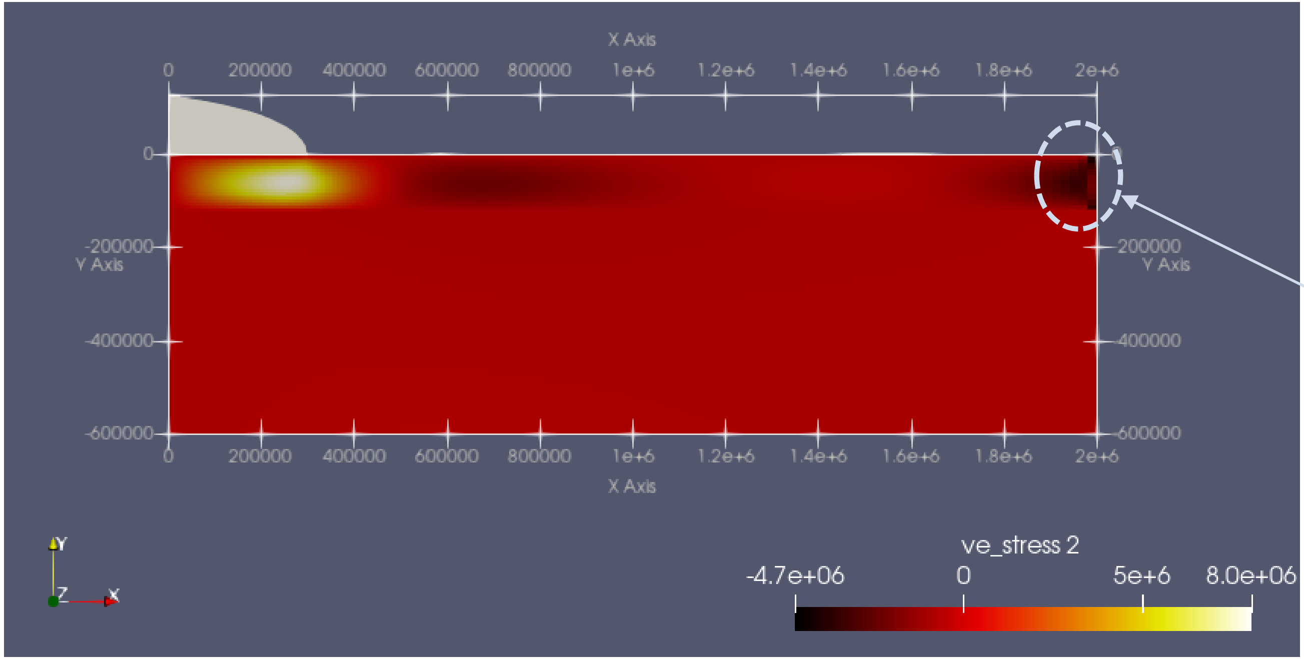


Coupled to ice sheet



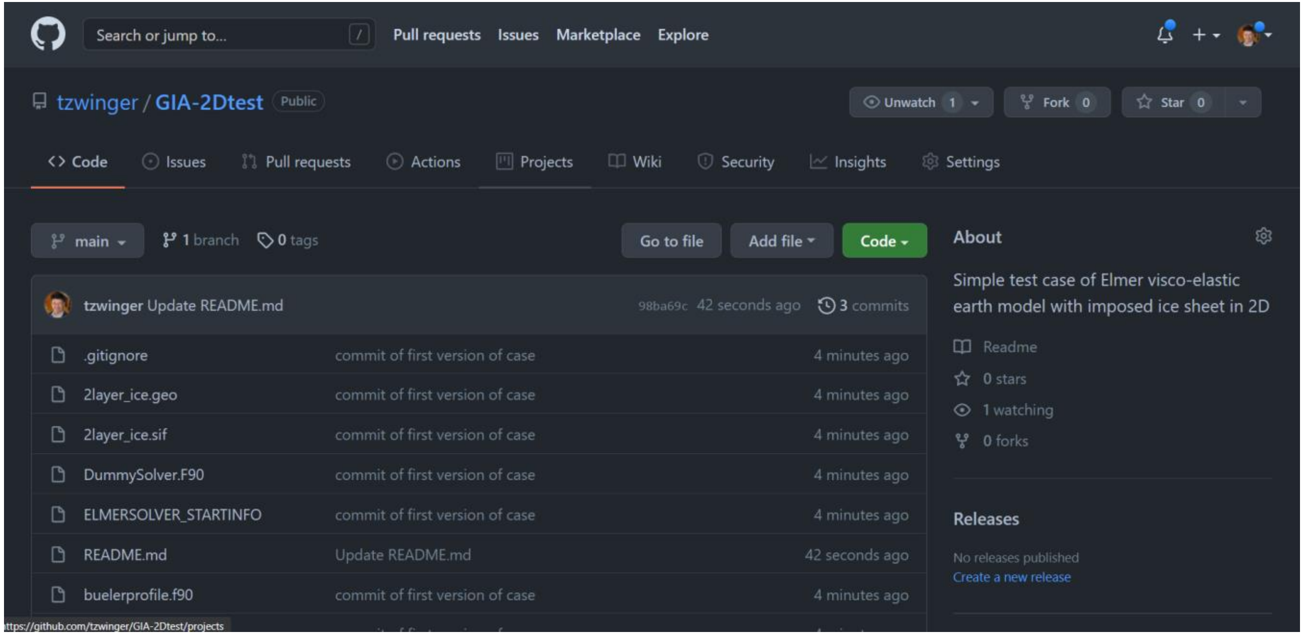
Far-field condition too close

Coupled to ice sheet



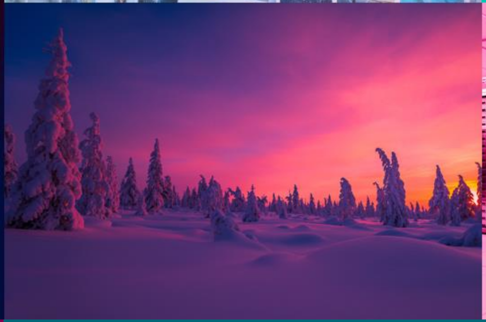
Far-field condition too close

Testcase to be found under GitHub: tzwinger/GIA-2Dtest



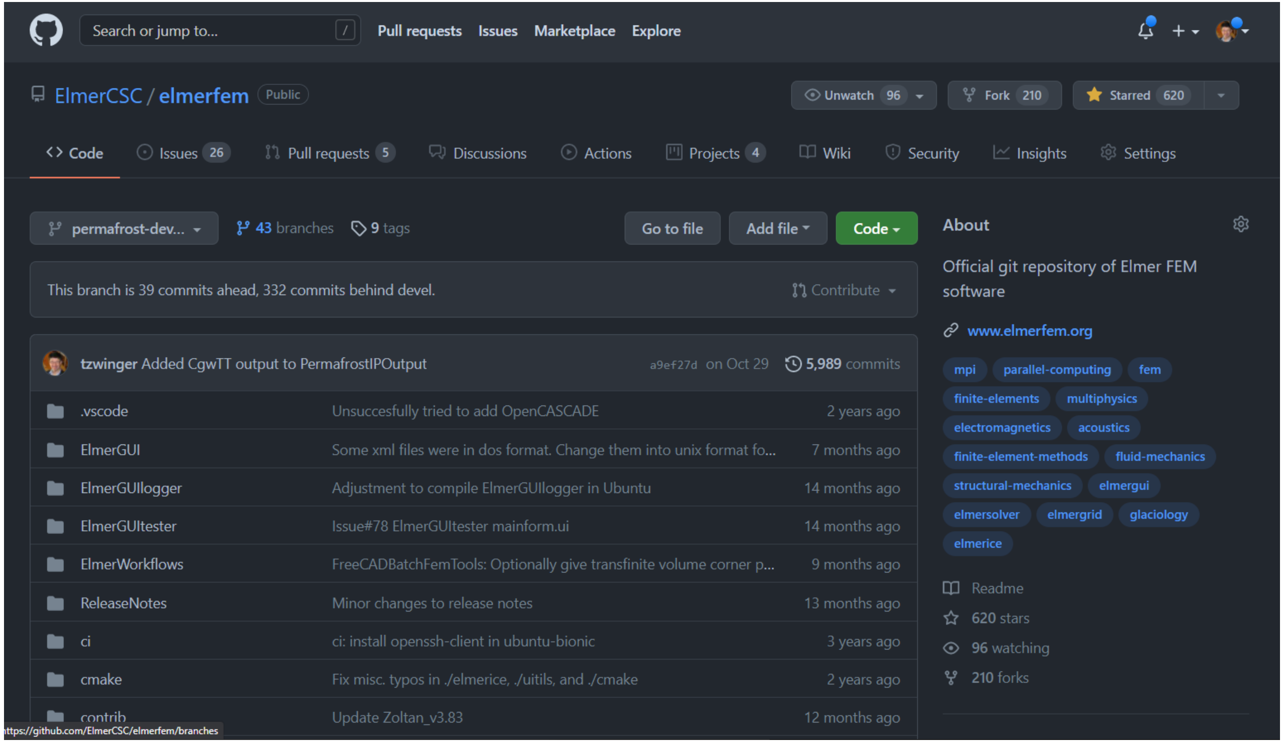
Groundwater-permafrost model






Groundwater-permafrost model

- This is still under heavy development
- Currently, special branch `permafrost-devel` in the GitHub repository is assigned to it



Permafrost model

- Implemented in the open-source software **Elmer**
  - Finite Element Method (standard Galerkin, plan for mixed elem.)
  - Easily coupled with **Elmer/Ice** ice-sheet simulation
  - Extra module with about 7000 lines of code
  - Main motivation: MPI/OpenMP parallelism (up to 1000's of cores)
- Each physical problem implemented in separate module
  - Fixed-point iterations on all other variables
  - Assumption of saturated aquifer
- Residual free bubbles for stabilization in case of advection
  - Potential to vectorise algorithm
- Dependent material parameters evaluated at IP's
  - Needed for accuracy
- p-elements of different orders

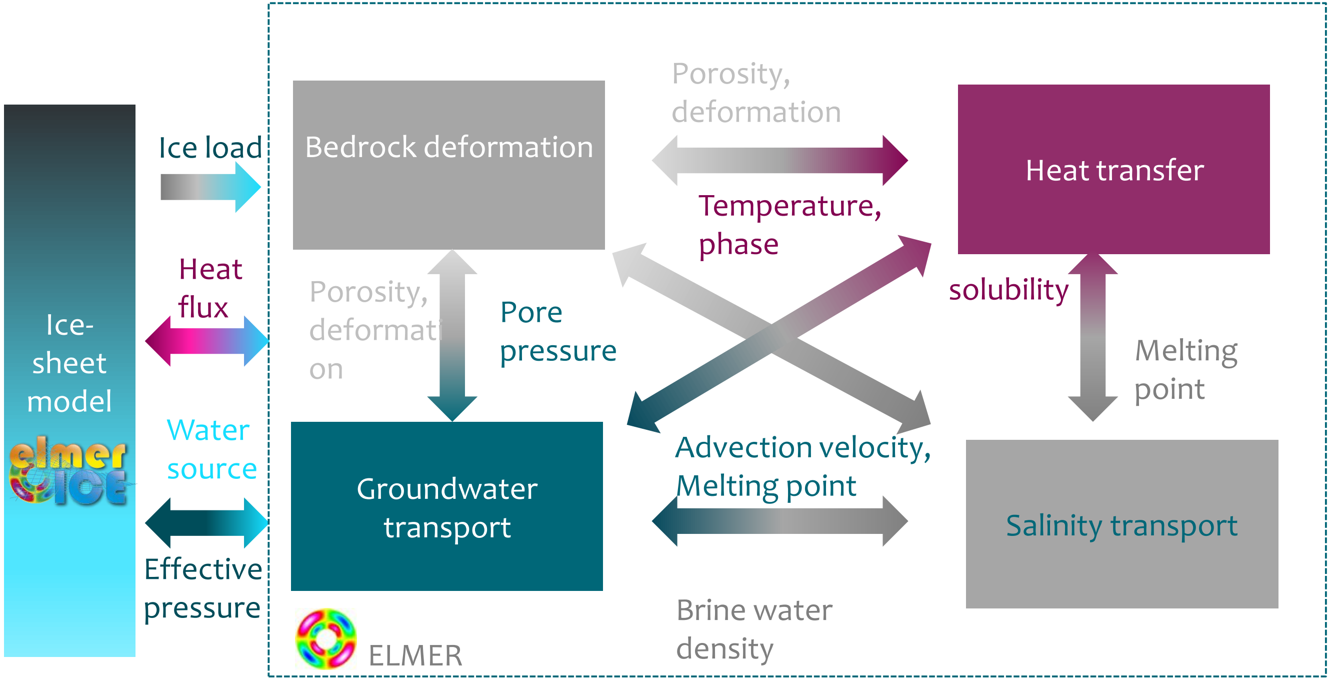
Heat transfer

Groundwater transport

Solute transport

Bedrock deformation

Permafrost model



Permafrost model

- Advection/Diffusion(/Reaction) type of equation

Groundwater transport

Advection Diffusion

Heat transfer

Solute transport

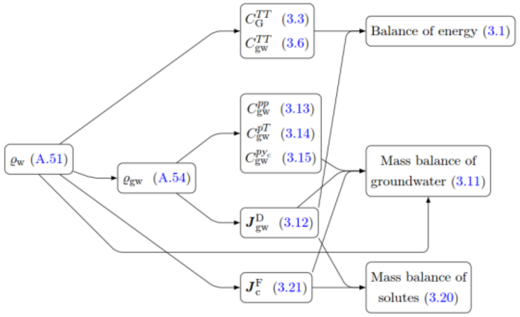
Bedrock deformation

$$C_{\mathrm{gw}}^{pp}\left(\frac{\partial p}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} p\right) + \operatorname{div}\left(\varrho_{\mathrm{gw}} \boldsymbol{J}_{\mathrm{gw}}^{\mathrm{D}}\right) + C_{\mathrm{gw}}^{pT}\left(\frac{\partial T}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} T\right) + \\ + C_{\mathrm{gw}}^{py_{\mathrm{c}}}\left(\frac{\partial y_{\mathrm{c}}}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} y_{\mathrm{c}}\right) + \operatorname{div}\left[\eta\left(\varrho_{\mathrm{c}} - \varrho_{\mathrm{w}}\right) \boldsymbol{J}_{\mathrm{c}}^{\mathrm{F}}\right] - C_{\mathrm{gw}}^{pI_1}\left(\frac{\partial I_1}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} I_1\right) = S_{\mathrm{gw}}.$$

Diffusion $\boldsymbol{J}_{\mathrm{gw}}^{\mathrm{D}} = -\left(\mathbf{K}_{\mathrm{gw}}^{pp} \cdot \operatorname{grad} p - \mathbf{K}_{\mathrm{gw}} \cdot \varrho_{\mathrm{gw}} \boldsymbol{g} + \mathbf{K}_{\mathrm{gw}}^{pT} \cdot \operatorname{grad} T\right).$

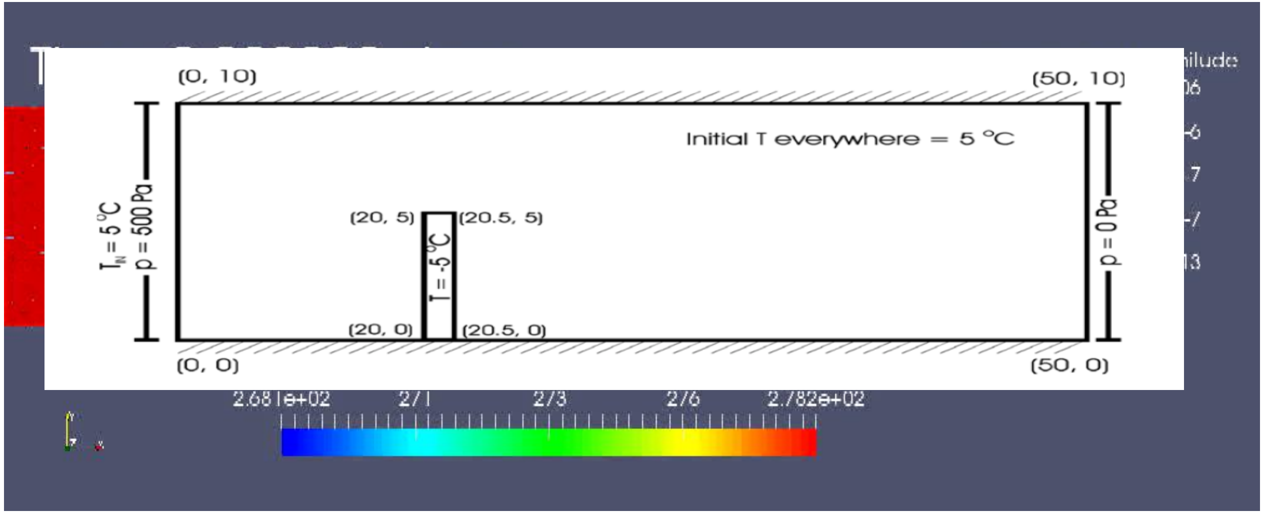
- High level of mutual dependencies (direct/indirect)

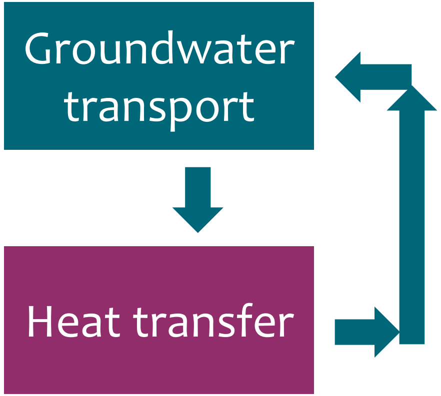
$$\varrho_{\mathrm{w}} = \varrho_{\mathrm{w0}} \exp\left[\kappa_{\mathrm{w0}}(p - p_0) - \alpha_{\mathrm{w0}}(T - T_0)\left(a_{\alpha_{\mathrm{w}},0} + \frac{1}{2} a_{\alpha_{\mathrm{w}},1} \frac{T - T_0}{T_0} + + \frac{1}{3} a_{\alpha_{\mathrm{w}},2}\left(\frac{T - T_0}{T_0}\right)^2 + \right.\right. \\ \left. + \frac{1}{4} a_{\alpha_{\mathrm{w}},3}\left(\frac{T - T_0}{T_0}\right)^3 + \frac{1}{5} a_{\alpha_{\mathrm{w}},4}\left(\frac{T - T_0}{T_0}\right)^4 + \frac{1}{6} a_{\alpha_{\mathrm{w}},5}\left(\frac{T - T_0}{T_0}\right)^5\right) + \\ \left. + \zeta_{\mathrm{w0}}\left(x_{\mathrm{w}} - x_{\mathrm{w0}}\right)\left(b_{\zeta_{\mathrm{w}},0} + \frac{1}{2} b_{\zeta_{\mathrm{w}},1}\left(x_{\mathrm{w}} - x_{\mathrm{w0}}\right)\right)\right], \quad \text{(A.51)}$$



Validation of single components

Coupled groundwater flow (after McKenzie at al., 2007)

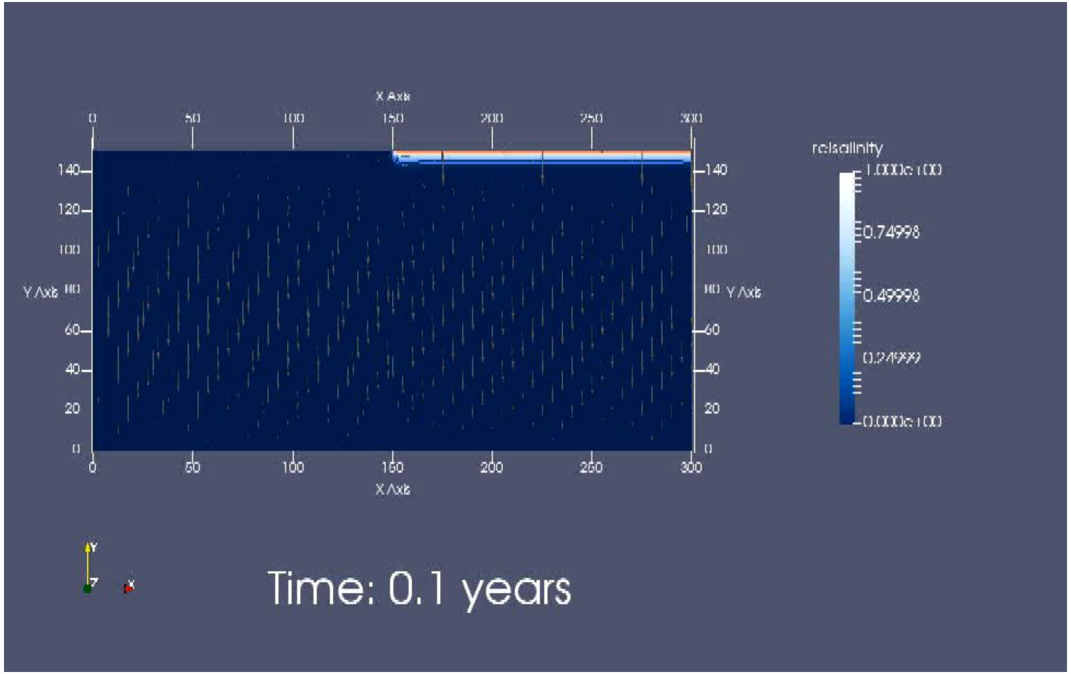


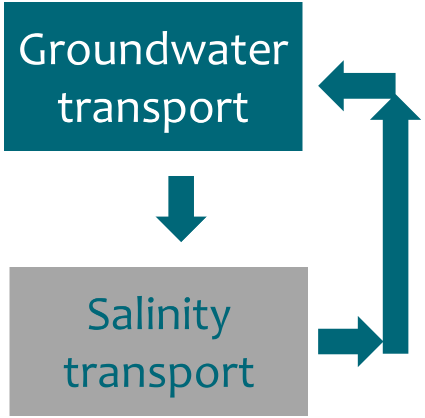


Simplified version of this experiment in source code: `elmerfem/elmerice/Tests/Permafrost_Frozenwall`

Validation of single components

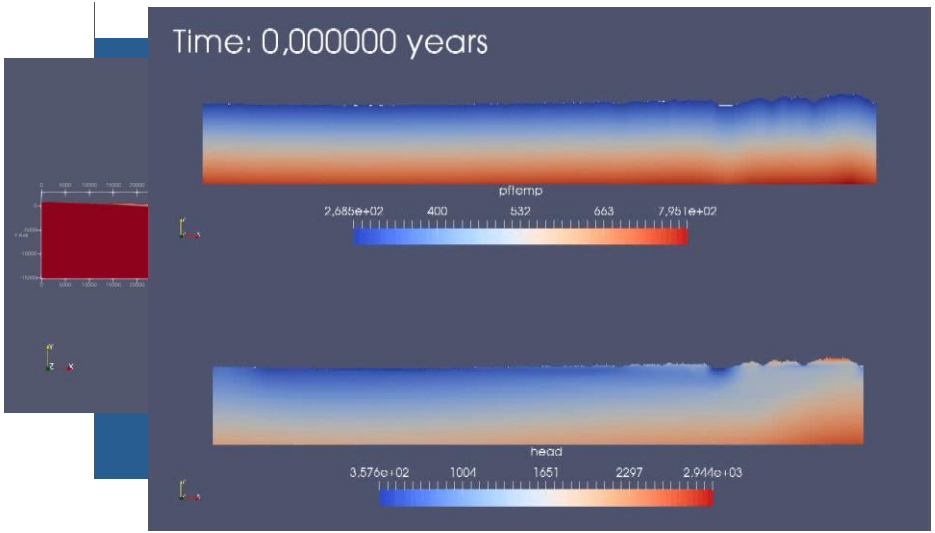
Elder Problem (Voss and Souza, 1987): salinity transport in porous medium



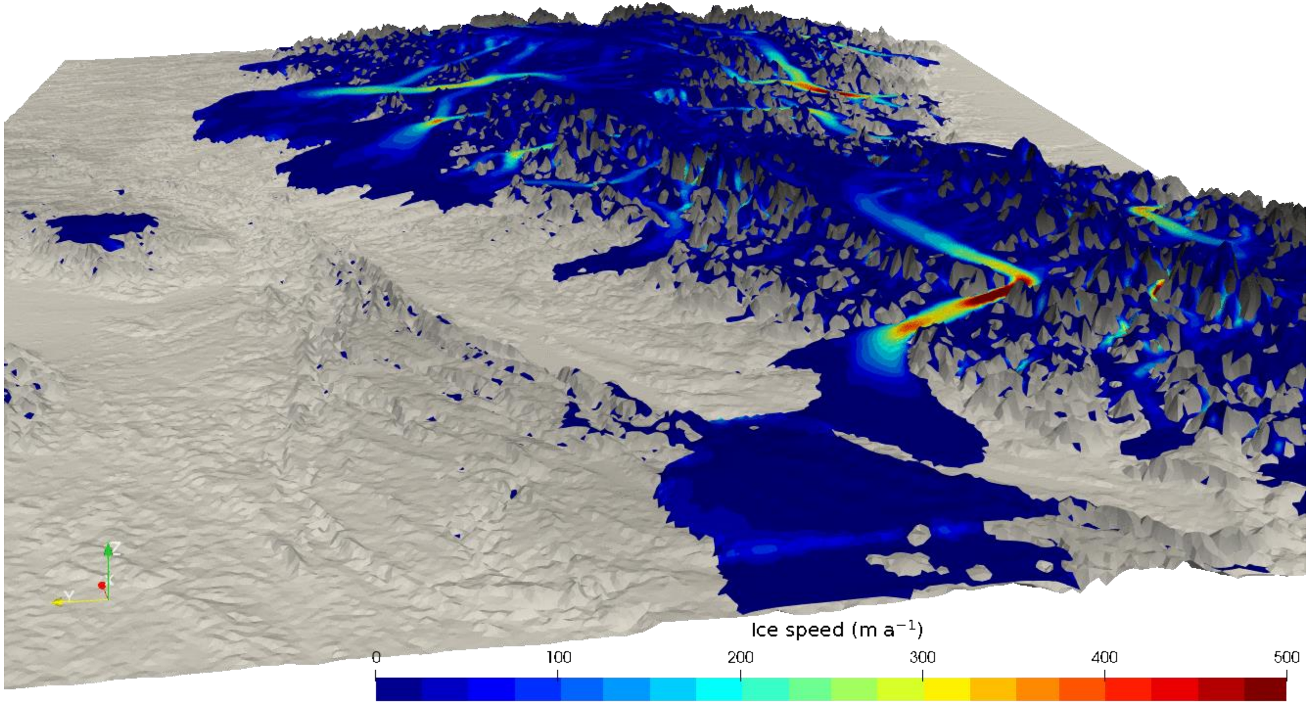


Nuclear waste repository safety assessment: Rhine Glacier

- Rhine Glacier simulation
- Flow-line along main branch
- Highly complex geology

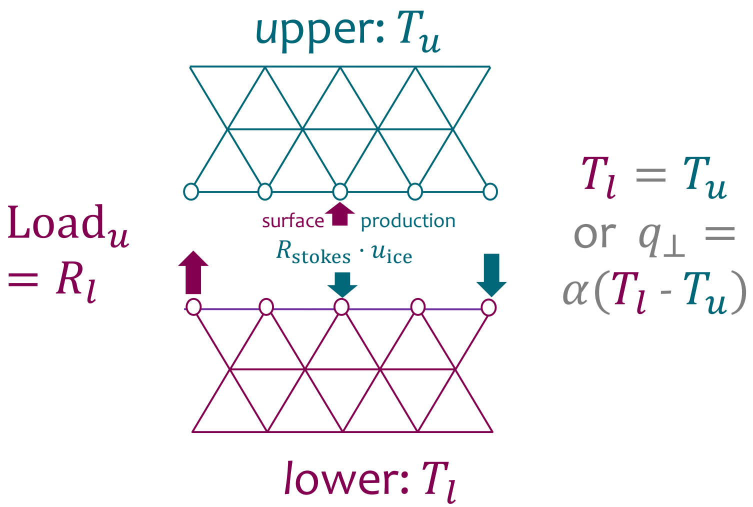


Nuclear waste repository safety assessment: Rhine Glacier

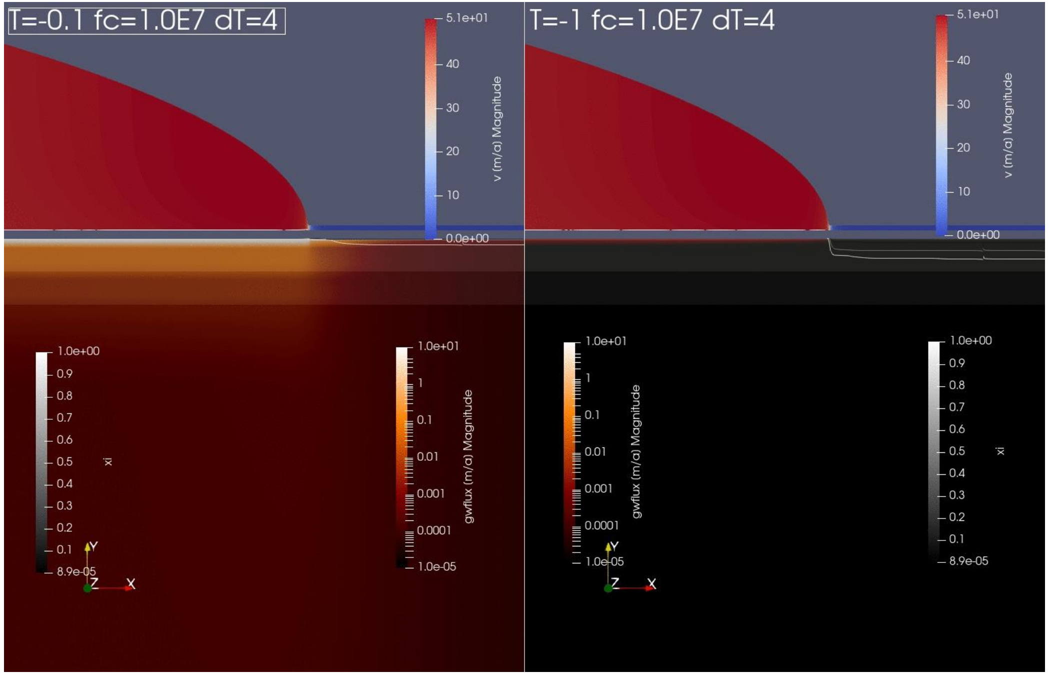


Coupling of ice-sheet to permafrost

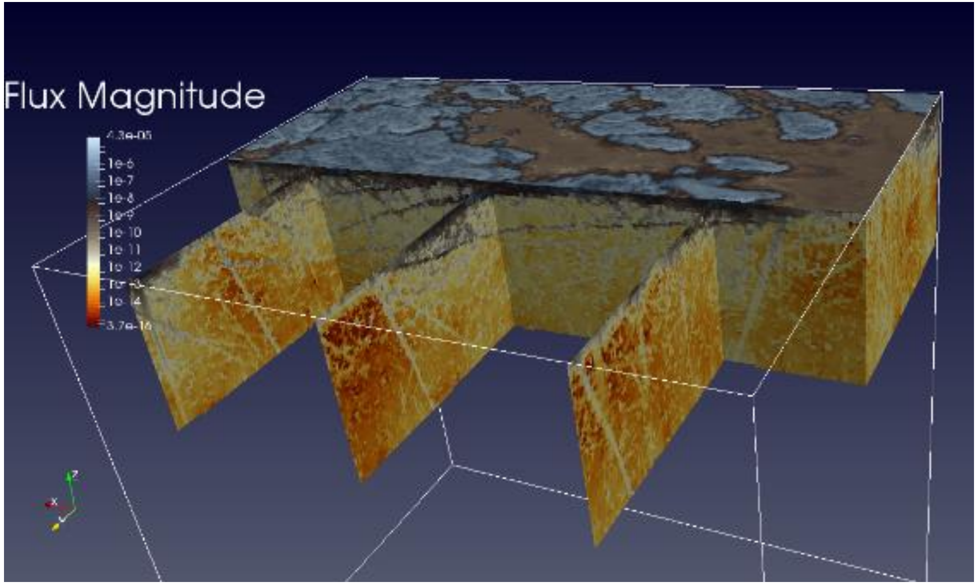
- Coupling of solver "of same kind" (e.g. Stokes and lin. Elasticity; HTEQ in ice and permafrost)
- Either Dirichlet-Neumann or Robin-Neumann
- Elegantly using residual as load
- Can also include surface production term



Coupling of ice-sheet to permafrost



Nuclear waste repository safety assessment: Olkiluoto



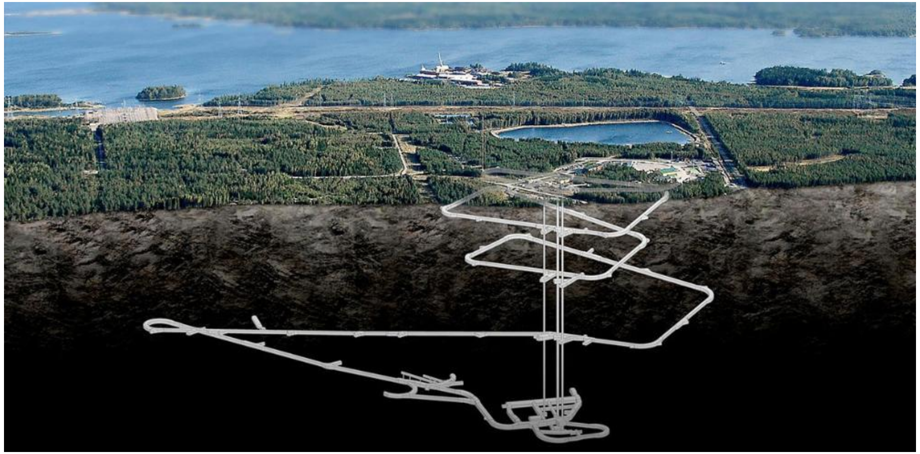
Posiva

Global leader in final disposal

Elmer

- Need to know future possible permafrost situation
- Development of high-fidelity groundwater/permafrost model
- 10x10x10 km^3 geological model around Olkiluoto – 30 m^3 resolution
- Outlook: include effects of approaching ice-sheet margin

Nuclear waste repository safety assessment: Olkiluoto



Source: Posiva.

- Need to know future possible permafrost situation
- Development of high-fidelity groundwater/permafrost model
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Nuclear waste repository safety assessment: Olkiluoto

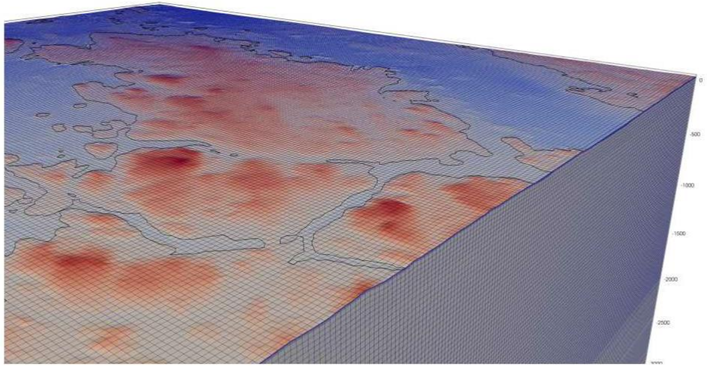


Figure 3: North-western corner of finite e lement m esh s howing regular 30 m × 30 m × 30 m discretization in the crystalline bedrock down to z = −2010 m, coarser discretization below (bottom right corner of figure), d iscretization i n t he soil layers. Horizontal discretization is uniform at. 30 m × 30 m.

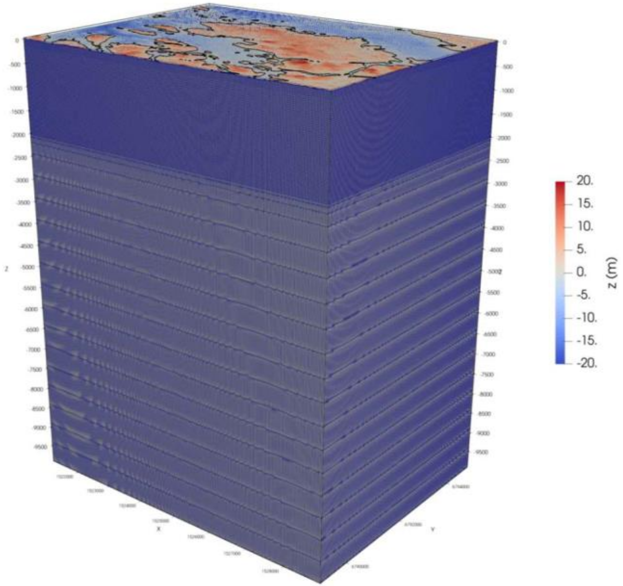


Figure 2: Three-dimensional model domain showing finite element mesh discretization.

Nuclear waste repository safety assessment: Olkiluoto

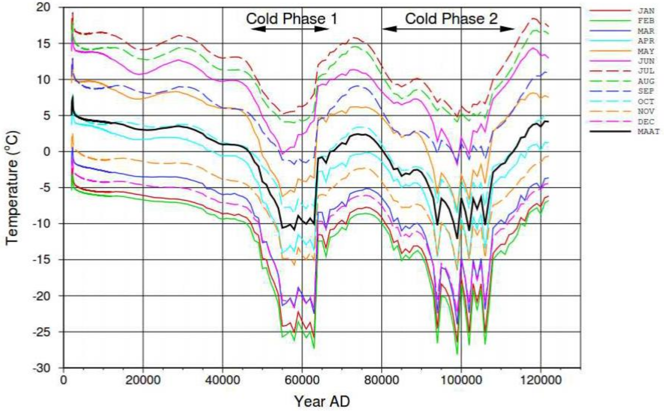


Figure 10: *Time series of monthly averaged and mean annual (MAAT) 2-meter air temperature for RCP4.5 Minimum Sea Level Scenario. Also indicated are the two cold phases, Cold Phase 1 and Cold Phase 2, identified by a MAAT less than zero degree Celsius.*

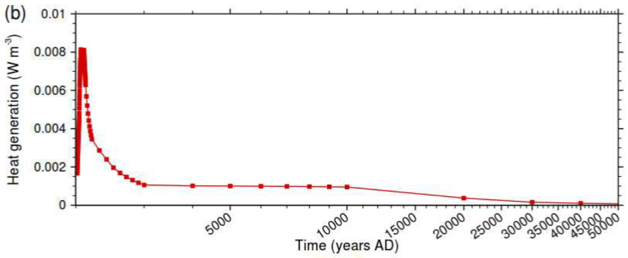


Figure 14: *Heat generation at Olkiluoto for Power Case 1 plotted with two different time scales: (a) linear and (b) using a logarithmic time scale.*

Nuclear waste repository safety assessment: Olkiluoto

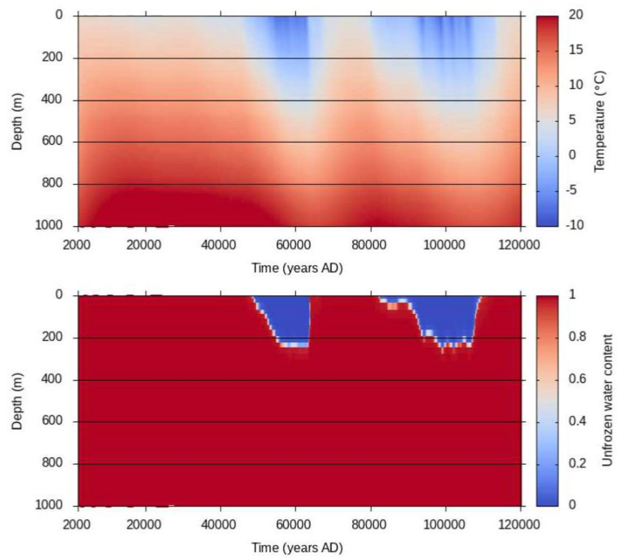


Figure 20: *Evolution of (top) temperature and (bottom) unfrozen water content (χ) at site 1 (see Figure 19), EPSG:2391 coordinate* 1,526,385 m, 6,792,340 m.

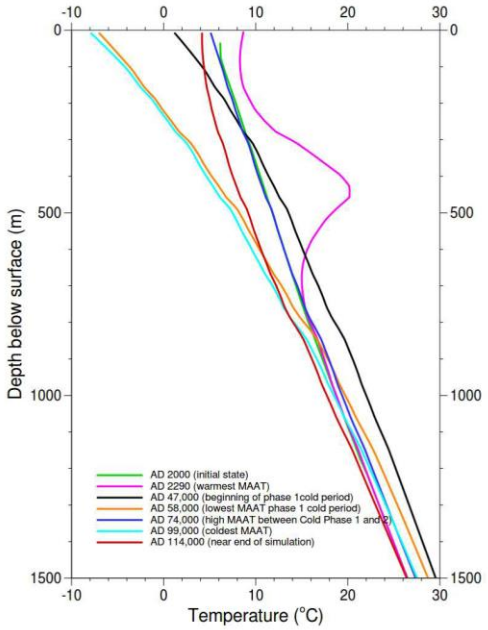


Figure 25: *Vertical temperature profile for site 3 down to a depth of* 1500 m *at various times during the simulation.*

Nuclear waste repository safety assessment: Olkiluoto

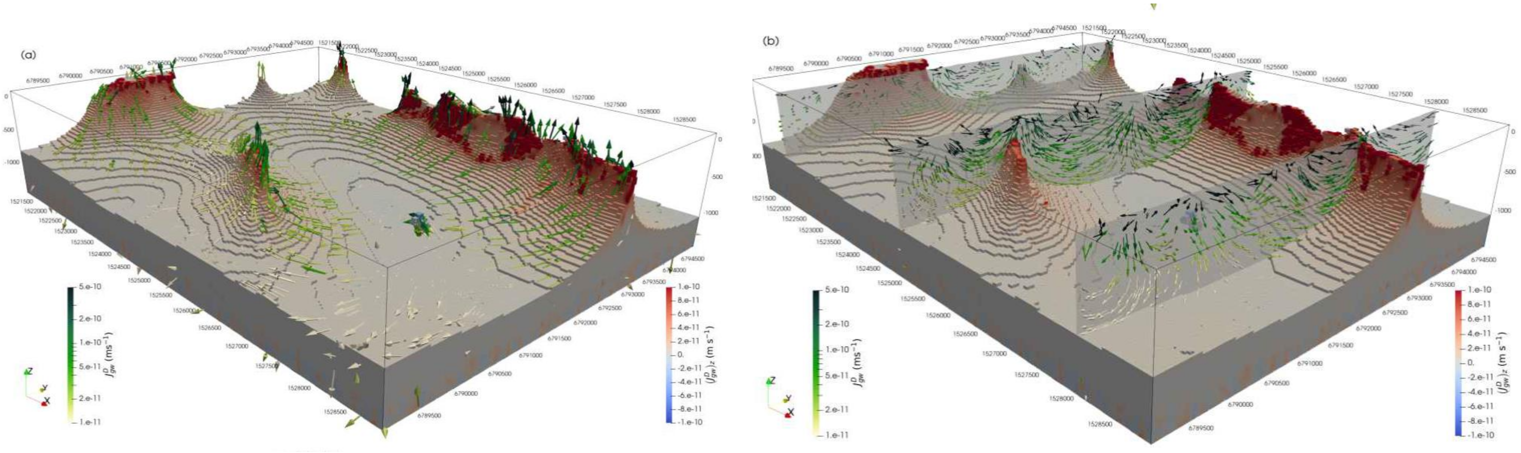
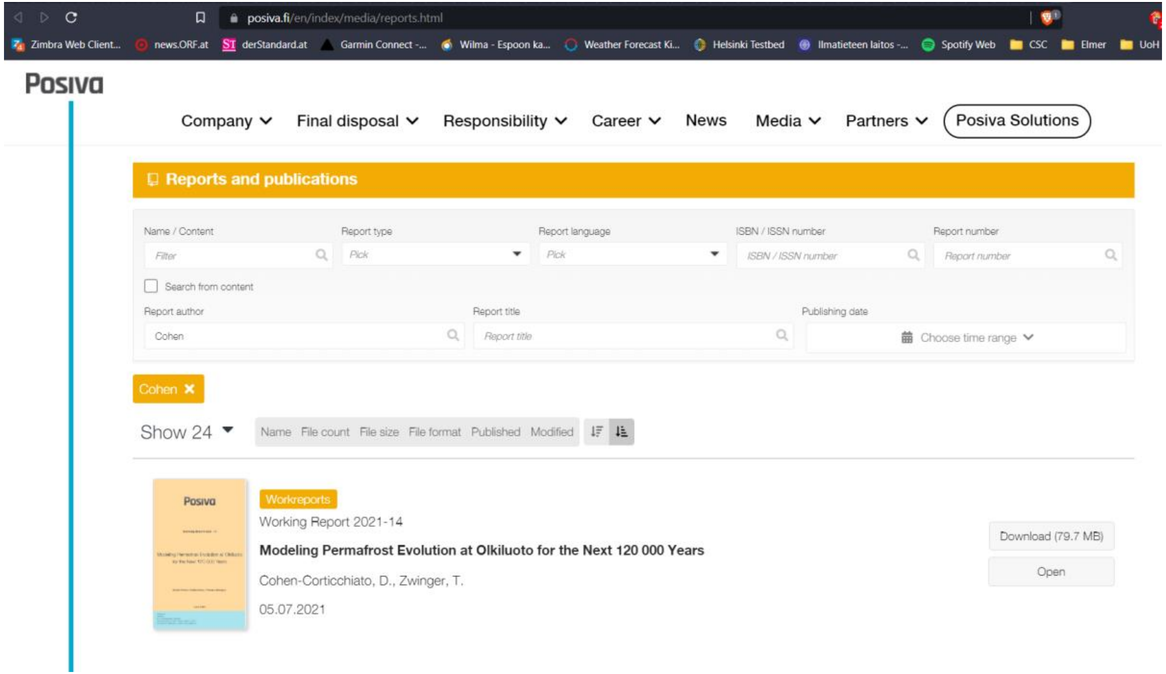
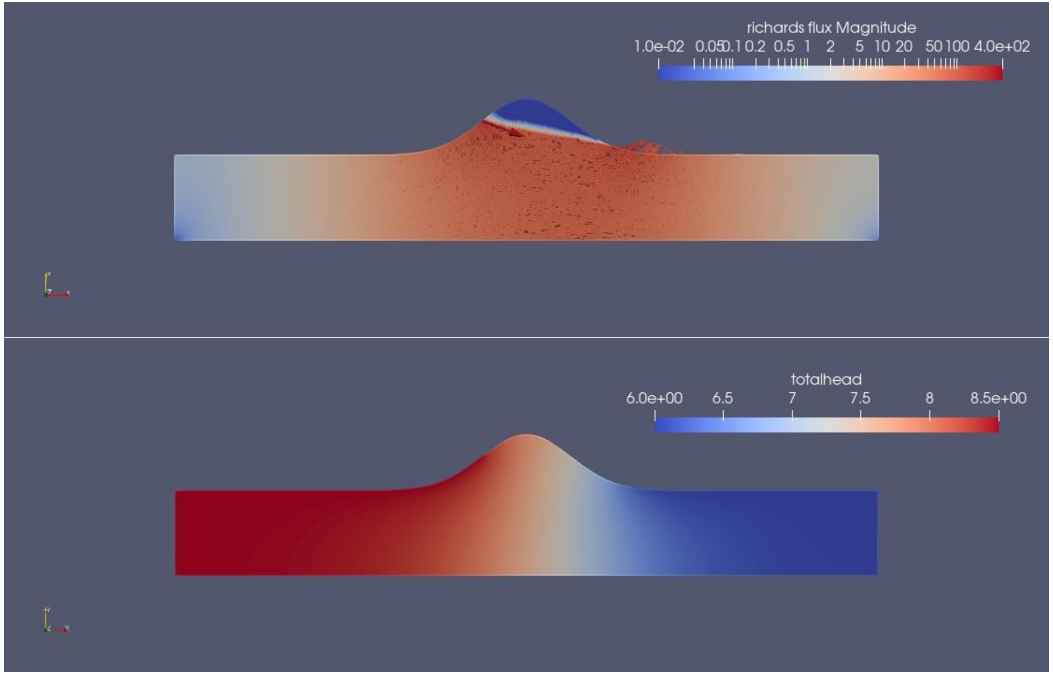


Figure 45: *Three dimensional block view at AD* 45,021 *before permafrost development of isosurface* $y_c = 2.0\ \mathrm{g\ L^{-1}}$ *showing groundwater flow vectors along (a) isosurface and (b) three vertical cross sections. Isosurface is colored according to vertical groundwater flux.*

Nuclear waste repository safety assessment: Olkiluoto



Richards equation for partly saturated aquifer (van Genuchten)



See Model 69 in Elmer Models Manual https://www.nic.funet.fi/pub/sci/physics/elmer/doc/ElmerModelsManual.pdf

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Additional material

Permafrost model

(T, p, y_c, η)

- Heat Transfer:

$$C_G^{TT}\left(\frac{\partial T}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} T\right) + C_{gw}^{TT} \operatorname{grad} T \cdot \boldsymbol{J}_{gw}^D + \operatorname{div} \boldsymbol{J}_G^H +$$
$$+ C_G^{Tp}\left(\frac{\partial p}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} p\right) + C_G^{Ty_c}\left(\frac{\partial T}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} y_c\right) = S_G$$

- Groundwater flow:

$$C_{gw}^{pp}\left(\frac{\partial p}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} p\right) + \operatorname{div}\left(\varrho_{gw} \boldsymbol{J}_{gw}^D\right) + C_{gw}^{pT}\left(\frac{\partial T}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} T\right) +$$
$$+ C_{gw}^{py_c}\left(\frac{\partial y_c}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} y_c\right) + \operatorname{div}\left[\eta\left(\varrho_c - \varrho_w\right) \boldsymbol{J}_c^F\right] - C_{gw}^{pI_1}\left(\frac{\partial I_1}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} I_1\right) = S_{gw},$$

- Solute transport:

$$C_c^{y_c y_c}\left(\frac{\partial y_c}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} y_c\right) + \operatorname{div}\left(\frac{y_c}{\chi} \varrho_c \boldsymbol{J}_{gw}^D\right) + \operatorname{div}\left(\eta \varrho_c \boldsymbol{J}_c^F\right) +$$
$$+ C_c^{y_c T}\left(\frac{\partial T}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} T\right) + C_c^{y_c p}\left(\frac{\partial p}{\partial t} + \boldsymbol{v}_* \cdot \operatorname{grad} p\right) = S_c$$

$$-\operatorname{div}\left(\boldsymbol{\sigma}^{ef} - p\mathbf{I}\right) = \rho_G \boldsymbol{g},$$

$$\boldsymbol{\sigma}^{ef} = \mathbb{C}_G : \boldsymbol{\epsilon} - \boldsymbol{\beta}_G (T - T_0)$$

Permafrost model

- Heat flux:

$$\boldsymbol{J}_{\mathrm{G}}^{\mathrm{H}} = -\mathbf{K}_{\mathrm{G}}^{TT} \cdot \operatorname{grad} T$$

- Groundwater flux:

$$\boldsymbol{J}_{\mathrm{gw}}^{\mathrm{D}} = -\left(\mathbf{K}_{\mathrm{gw}}^{pp} \cdot \operatorname{grad} p - \mathbf{K}_{\mathrm{gw}} \cdot \varrho_{\mathrm{gw}} \boldsymbol{g} + \mathbf{K}_{\mathrm{gw}}^{pT} \cdot \operatorname{grad} T\right).$$

- Solute flux:

$$\boldsymbol{J}_{\mathrm{c}}^{\mathrm{F}} = -\left(\mathbf{K}_{\mathrm{c}}^{y_{\mathrm{c}} y_{\mathrm{c}}} \cdot \operatorname{grad} y_{\mathrm{c}} - \mathbf{K}_{\mathrm{c}} \cdot \boldsymbol{f}_{\mathrm{c}} \, y_{\mathrm{c}}\right)$$

- Elasticity tensor:

$$\mathbf{K}_{\mathrm{G}}^{\boldsymbol{uu}} = \frac{E_{\mathrm{G}}}{(1+\nu_{\mathrm{G}})(1-2\nu_{\mathrm{G}})} \begin{bmatrix} 1-\nu_{\mathrm{G}} & \nu_{\mathrm{G}} & \nu_{\mathrm{G}} & 0 & 0 & 0 \\ \nu_{\mathrm{G}} & 1-\nu_{\mathrm{G}} & \nu_{\mathrm{G}} & 0 & 0 & 0 \\ \nu_{\mathrm{G}} & \nu_{\mathrm{G}} & 1-\nu_{\mathrm{G}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu_{\mathrm{G}}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu_{\mathrm{G}}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu_{\mathrm{G}}}{2} \end{bmatrix},$$

$$E_{\mathrm{G}} = (1-\eta)\frac{E_{\mathrm{s},0}}{1-\eta_0} + \eta(1-\chi)E_{\mathrm{i}},$$

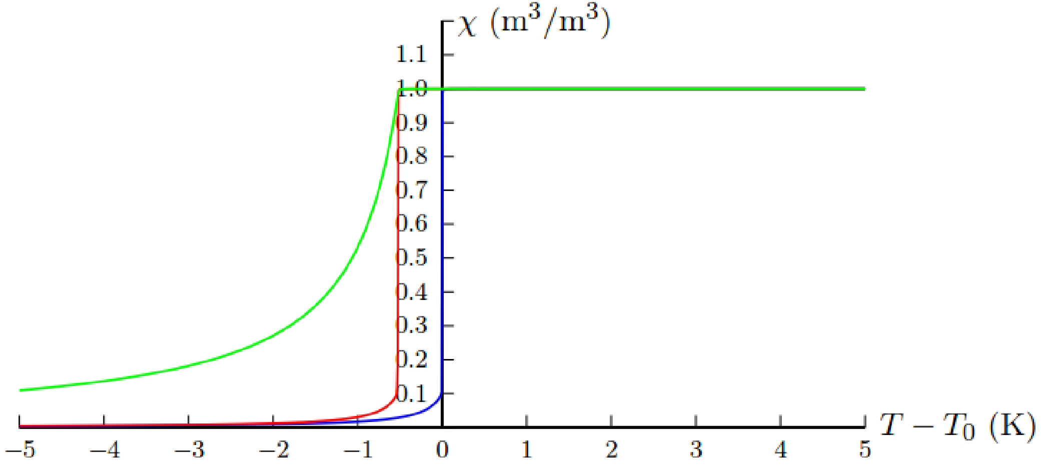
$$\nu_{\mathrm{G}} = (1-\eta)\nu_{\mathrm{s},0} + \eta(1-\chi)\nu_{\mathrm{i}}.$$

Permafrost model

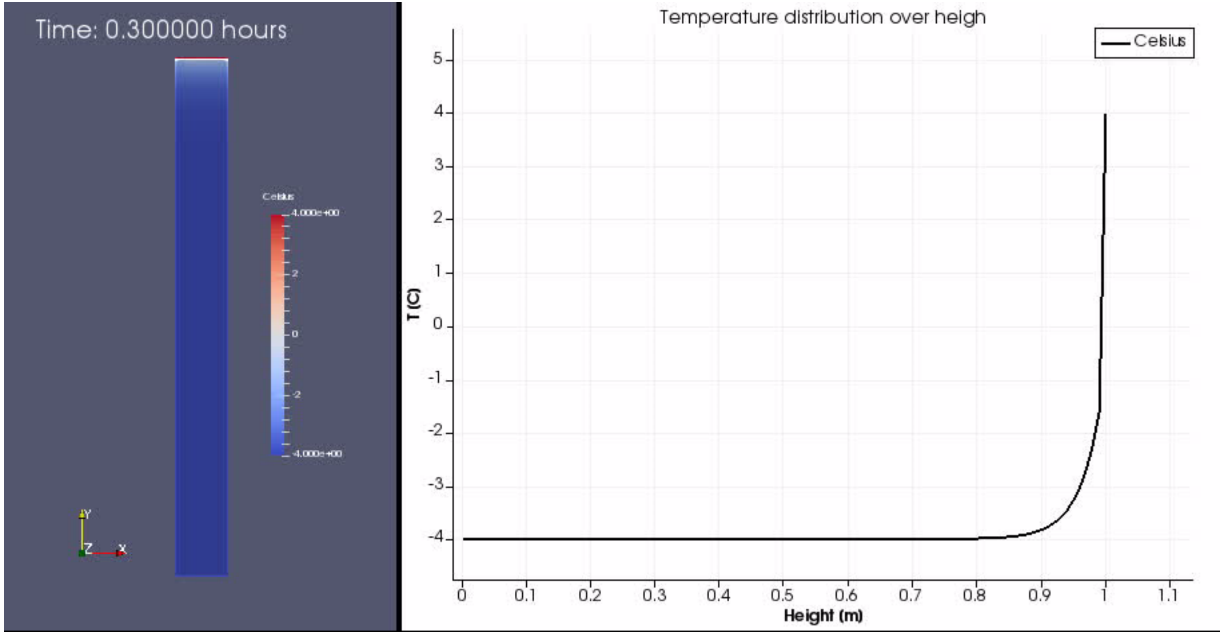
- Phase change: Frozen water content [0,1]

$$\chi = \chi(T, p, y_c, \eta)$$

$$y_c = \chi \cdot x_c,$$



Validation of single components



Heat transfer

Stefan Problem: freezing/thawing front in water column