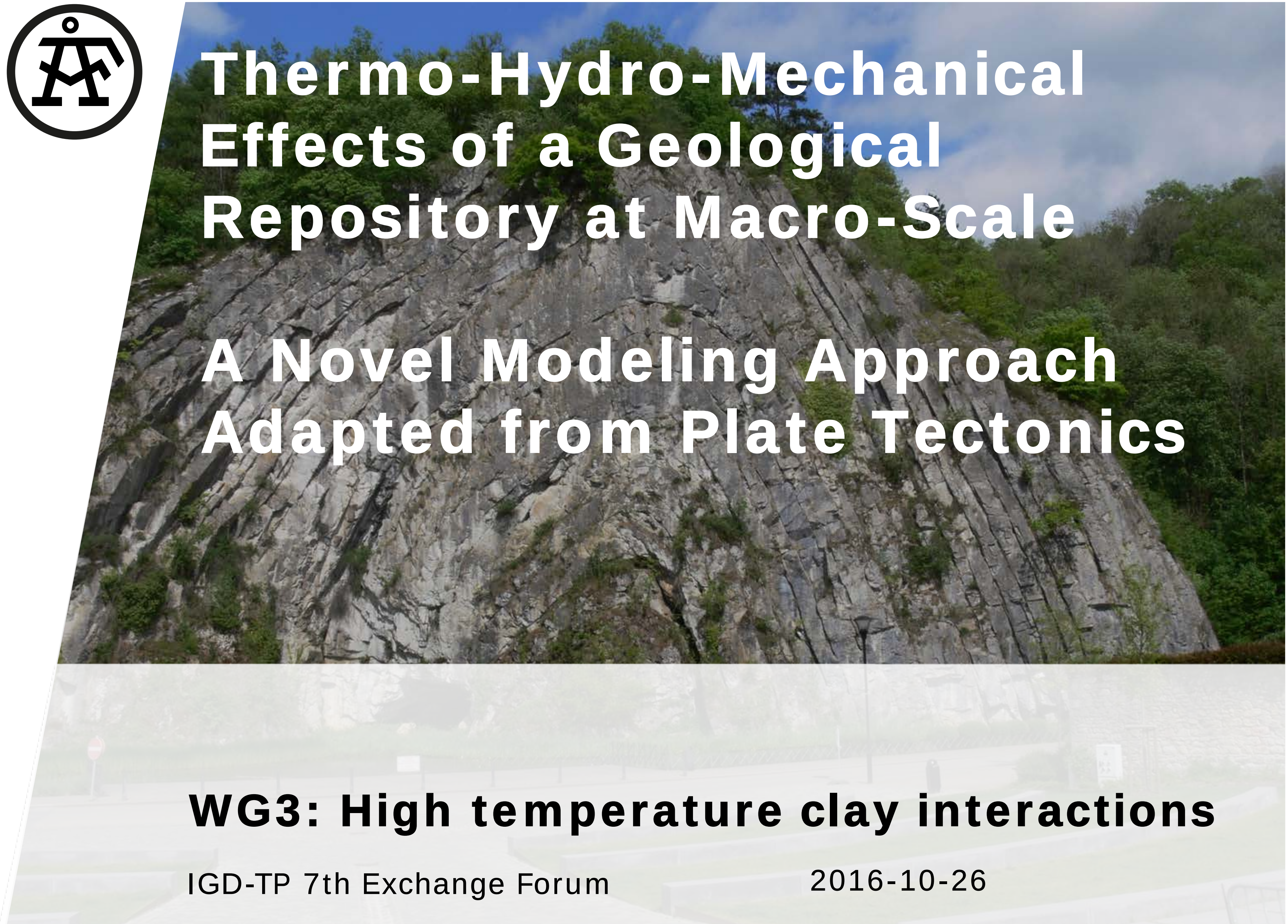


Thermo-Hydro-Mechanical Effects of a Geological Repository at Macro-Scale

A Novel Modeling Approach Adapted from Plate Tectonics

WG3: High temperature clay interactions

IGD-TP 7th Exchange Forum

2016-10-26

Content

- Introduction, objectives
- Approach used in geodynamics & plate tectonics
- Scope of the work
- Adapted system of equations
- Numerical implementation
- Test 2D simulation and results
- Conclusions and next steps

Introduction / Objectives

In repositories, heat generated from the high active waste may affect the near and far field:

- Heat diffuses (and may advectively be transported), which induces
- Thermal expansion of skeleton and pore water
- Pressure build-up and impact on stresses
- Fracturing may result

Dimensioning of repositories is sensibly constrained by these THM effects.

Various THM modelling approaches have been investigated and applied in the context of radioactive waste. Large scale modelling remains a challenge.

In geodynamics modelling THM phenomena e.g., in subduction zones, is also a challenge.

Objective: Assess methods used in computational geodynamics and plate tectonics and investigate whether the modelling approach could be applied to THM physics of a geological repository in clay host rock.

One Approach used in Geodynamics & Plate Tectonics

- Modeling subduction as a 2-phase flow: solid-fluid
- Governing equations for (de)compacting visco-plastic incompressible solid and incompressible fluid:

- Total momentum conservation (in the solid velocity frame)

$$\frac{\partial \sigma'_{ij}}{\partial x_j} - \frac{\partial p_t}{\partial x_i} = -g_i \rho_t,$$

- Mass conservation of the solid

$$div(v^S) = -\frac{p_t - p_f}{\eta_{bulk}}$$

- Fluid momentum conservation (Darcy)

$$v_y^D = \frac{K}{\eta_f} \cdot \left(\rho_f g_y - \frac{\partial p_f}{\partial y} \right)$$

- Mass conservation of fluid

$$div(v^D) = \frac{p_t - p_f}{\eta_{bulk}}$$

- Matrix porosity evolution

$$\frac{D \ln(1-\varphi)}{Dt} = \frac{p_t - p_f}{\eta_{bulk}}$$

- Brittle/plastic deformation (and grain friction within the solid)

$\sigma_{yield} = C + \gamma(p_t - p_f)$

γ=0-0.85 for $p_t > p_f$ (confined fractures)

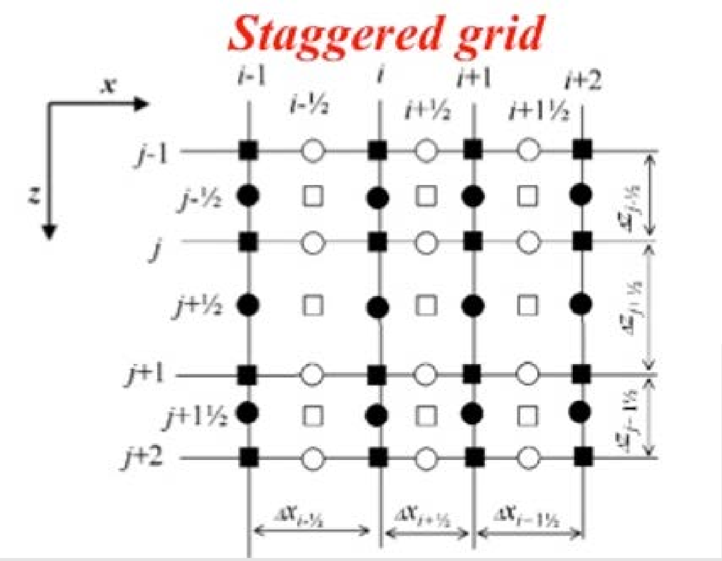
γ=1 for $p_t < p_f$ (tensile fractures)

(Dymkova and Gerya, 2013, supplement)

One Approach used in Geodynamics & Plate Tectonics

A fast method for numerical simulation

- Combination of finite differences, on staggered grid

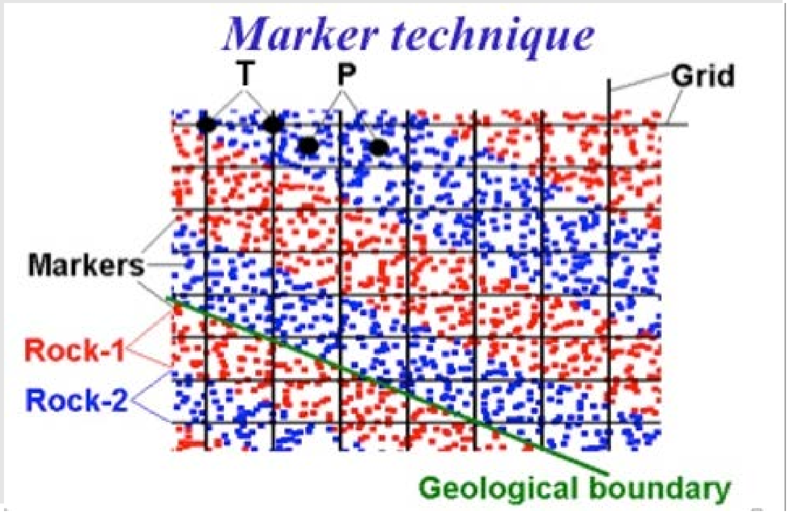


Variables

- ● v_x, ρ, K
- ○ v_z, ρ, K
- ■ ε_{xz}, σ_{xz}, η
- □ P, ε_{xx}, ε_{zz}, σ_{xx}, σ_{zz}, η, η_{bulk}

- And moving marker technique

  Markers holds physical properties of the (moving) materials which are interpolated to the grid nodes



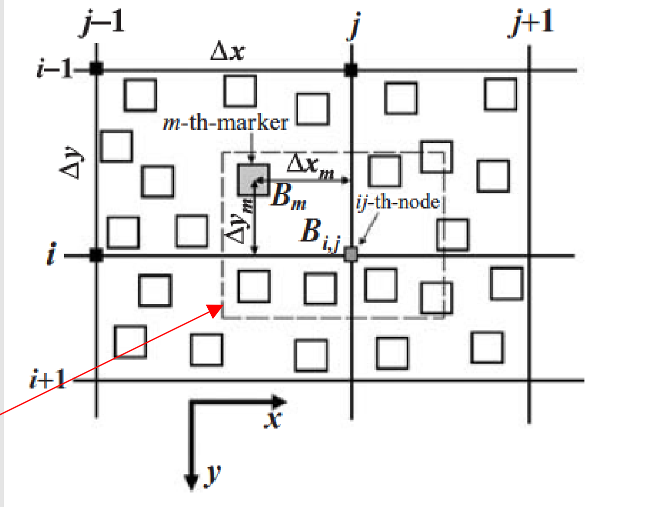
One Approach used in Geodynamics & Plate Tectonics

Markers <-> node interpolation for a property *B* at node *i,j*:

- *Markers -> nodes*

$$B_{i,j} = \frac{\sum_m B_m w_{m(i,j)}}{\sum_m w_{m(i,j)}},$$

$$w_{m(i,j)} = \left(1 - \frac{\Delta x_m}{\Delta x}\right) \times \left(1 - \frac{\Delta y_m}{\Delta y}\right)$$

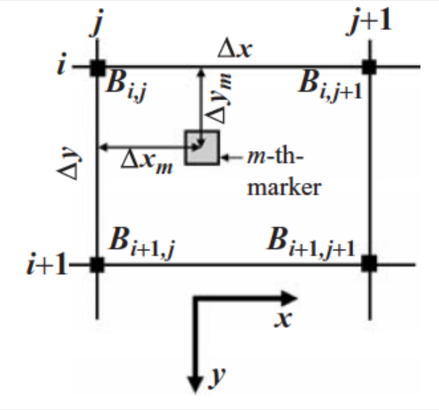


Area from which markers *m* holding properties B_m are used for interpolation at node (*i,j*) – local interpolation scheme

- *Nodes -> markers*

$$B_m = B_{i,j}\left(1 - \frac{\Delta x_m}{\Delta x}\right)\left(1 - \frac{\Delta y_m}{\Delta y}\right) + B_{i,j+1}\frac{\Delta x_m}{\Delta x}\left(1 - \frac{\Delta y_m}{\Delta y}\right)$$

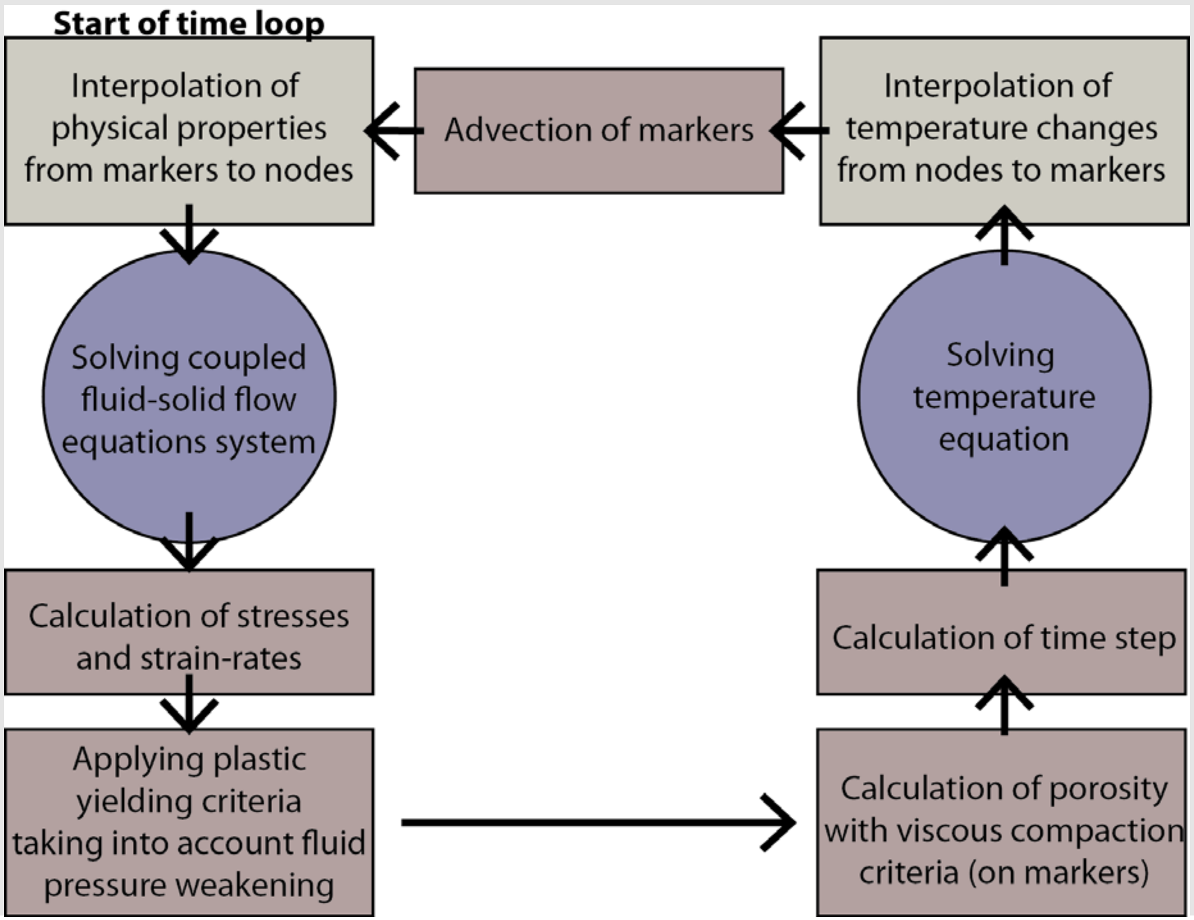
$$+ B_{i+1,j}\left(1 - \frac{\Delta x_m}{\Delta x}\right)\frac{\Delta y_m}{\Delta y} + B_{i+1,j+1}\frac{\Delta x_m \Delta y_m}{\Delta x \Delta y},$$



(Gerya, 2010)

One Approach used in Geodynamics & Plate Tectonics

Numerical algorithm for the finite differences, on staggered grid with marker technique



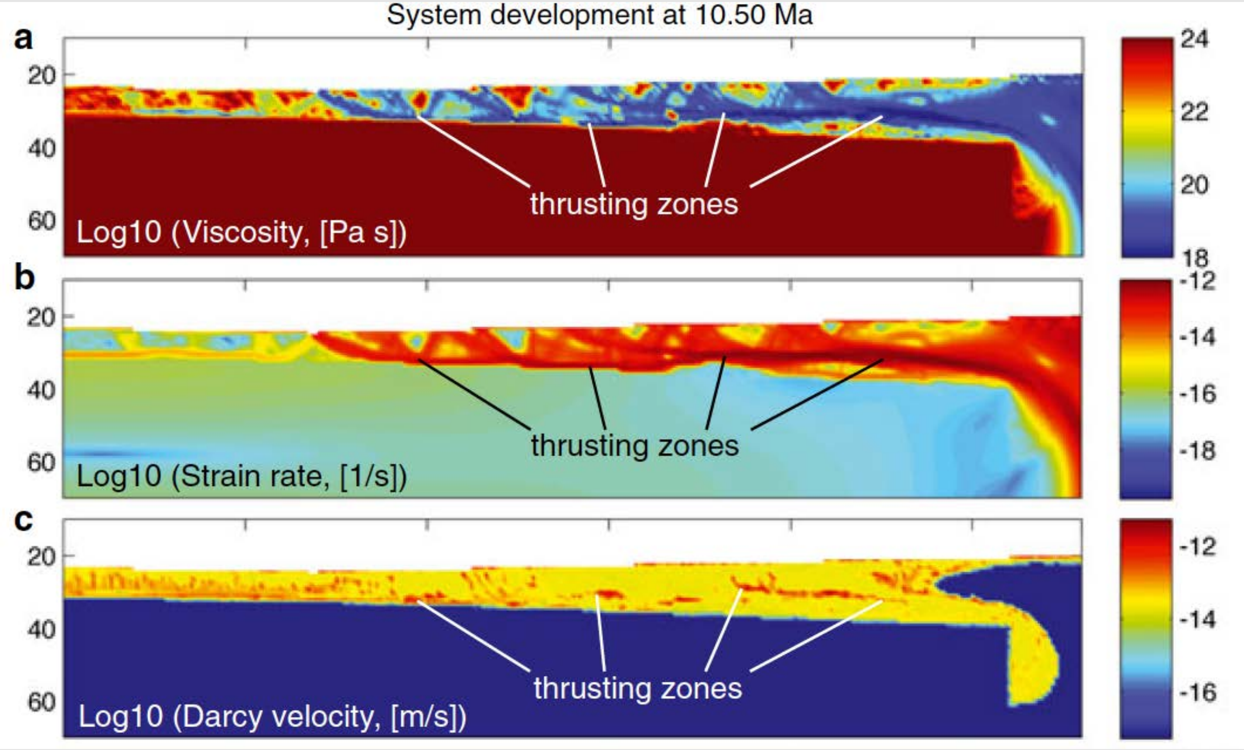
(Dymkova, 2014, PhD thesis)

One Approach used in Geodynamics & Plate Tectonics

Numerical application: Water-induced faulting of rocks:

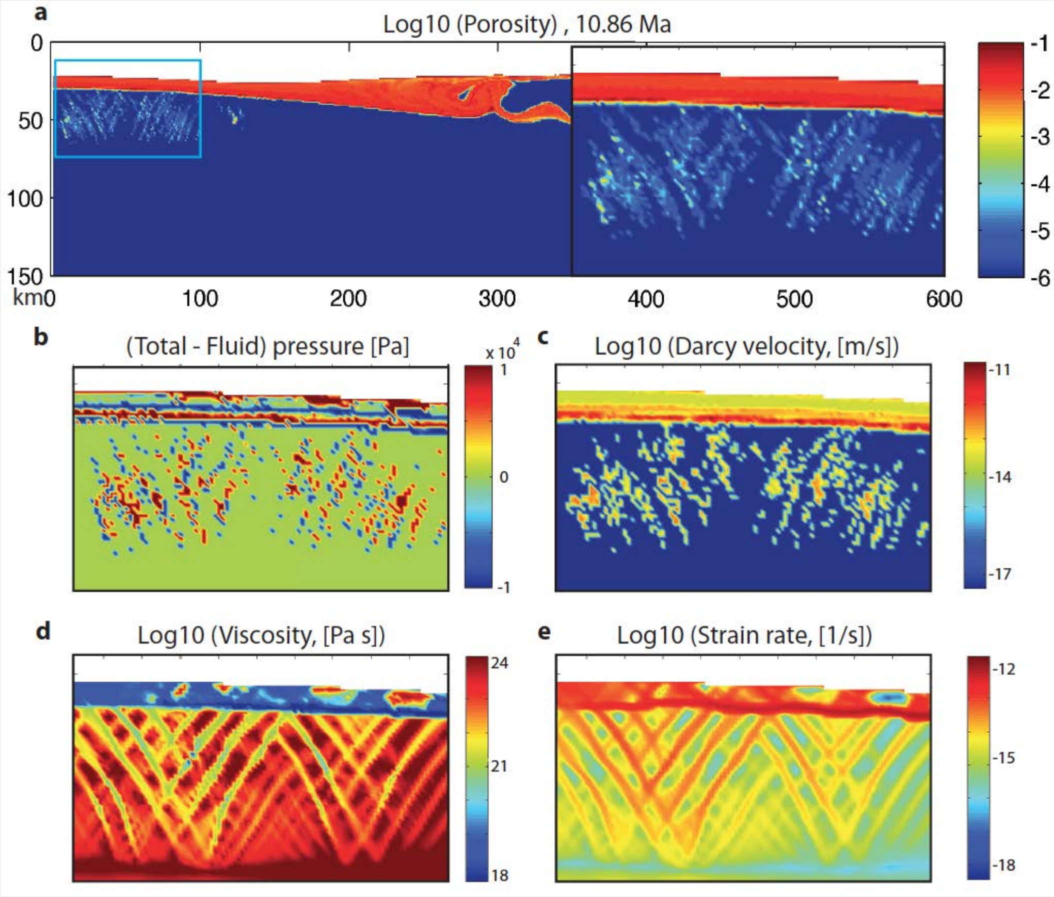
During spontaneous subduction initiation, pressurized fluid percolation is localized along multiple listric propagating thrusts.

Their coalescing roots form incipient hydrated subduction interface.



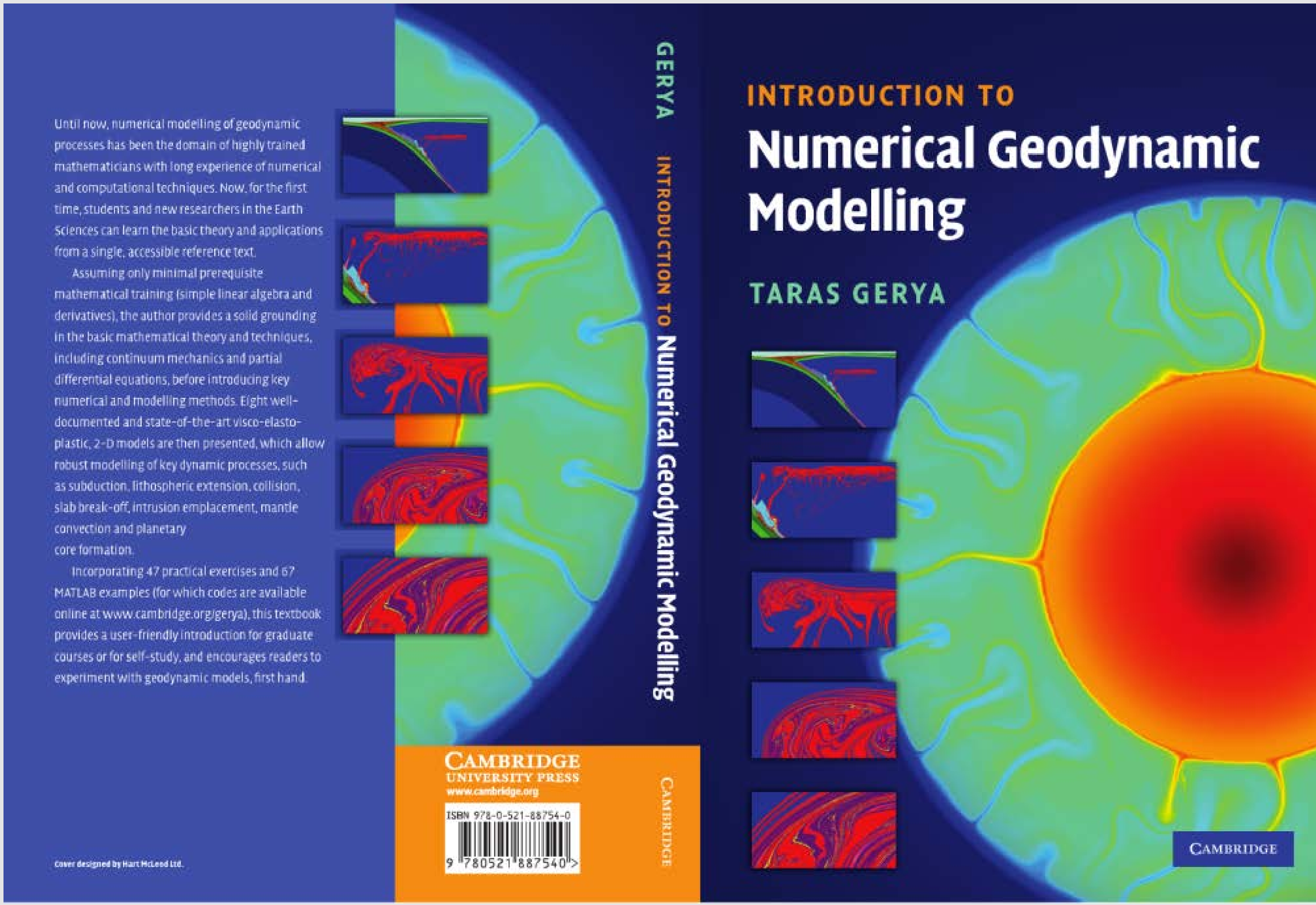
One Approach used in Geodynamics & Plate Tectonics

Numerical application: Downward water suction by deviatoric stresses in the bending subducting plate



(Dymkova and Gerya, 2013)

More on Geodynamics & Plate Tectonics…



Scope of Work

- Derive from the Geodynamics approach a model suitable for THM problems in radwaste repositories with:
  - Thermal including heat source stemming from radioactive decay

    (T – HM approached: T is decoupled)
  - Visco-elasto-plastic material behaviour
  - Compressibility of the fluid and solid phase
  - Saturated host rock

- Implement a proof of concept and test the approach on a simple case to verify its ability to numerically resolve the problem

Adapted System of Equations

- Energy conservation

$$\rho C_P\left(\frac{DT}{Dt}\right) = \nabla\cdot(k\nabla T) + H$$

With $H = H_r + H_a + H_s$

- Hr = source term New
- $H_a = T\alpha\frac{DP}{Dt}$
- $H_s = \sigma'_{ij}\dot{\varepsilon}'_{ij}$

- Porosity evolution

$$\frac{D\ln(1-\phi)}{Dt} = \frac{P_eff}{\zeta} - \frac{\phi\,(\beta_b-\beta_p)}{1-\phi}\frac{DP_{eff}}{Dt}$$

$$P_{eff} = P - P_f$$

- Compressible HM equations
  - Momentum $\nabla\cdot\sigma' - \nabla P + \rho\vec{g} = 0$
  - Mass conservation solid, fluid

$$\nabla\cdot\vec{v}_s + \frac{P_eff}{\zeta} = \frac{\phi\,(\beta_b-\beta_p)}{1-\phi}\frac{DP_{eff}}{Dt} - \frac{D\ln(\rho_s)}{Dt}$$

New

$$\nabla\cdot\vec{v}_D - \frac{P_eff}{\zeta} = \frac{\phi\,(\beta_b-\beta_p)}{1-\phi}\frac{DP_{eff}}{Dt} - \phi\frac{D\ln(\rho_f)}{Dt} + \phi\frac{D\ln(\rho_s)}{Dt}$$

New

- Fluid momentum conservation (Darcy)

$$\vec{v}_D + \frac{K}{\eta_f}\nabla P_f = \frac{K}{\eta_f}\rho_f\vec{g}$$

Where

$$\sigma'_{ij} = 2\eta\dot{\varepsilon}'_{ij}Z + \sigma'^{0}_{ij}(1-Z)$$

$$Z = \frac{\mu dt}{\mu dt + \eta}$$

New

$$\rho_s = \rho_{s(r)}\exp(\beta(P - P_(r)) - \alpha(T - T_(r)))$$

$$\rho_f = \rho_{f(r)}\exp(\beta(P - P_(r)) - \alpha(T - T_(r)))$$

$$\sigma'_{ij} = 2\eta\dot{\varepsilon}'_{ij} + \delta_{ij}\zeta\dot{\varepsilon}_{kk}$$

$$\dot{\varepsilon}'_{ij} = \frac{1}{2}\left(\frac{\partial v_i^s}{\partial x_j} + \frac{\partial v_j^s}{\partial x_i}\right)$$

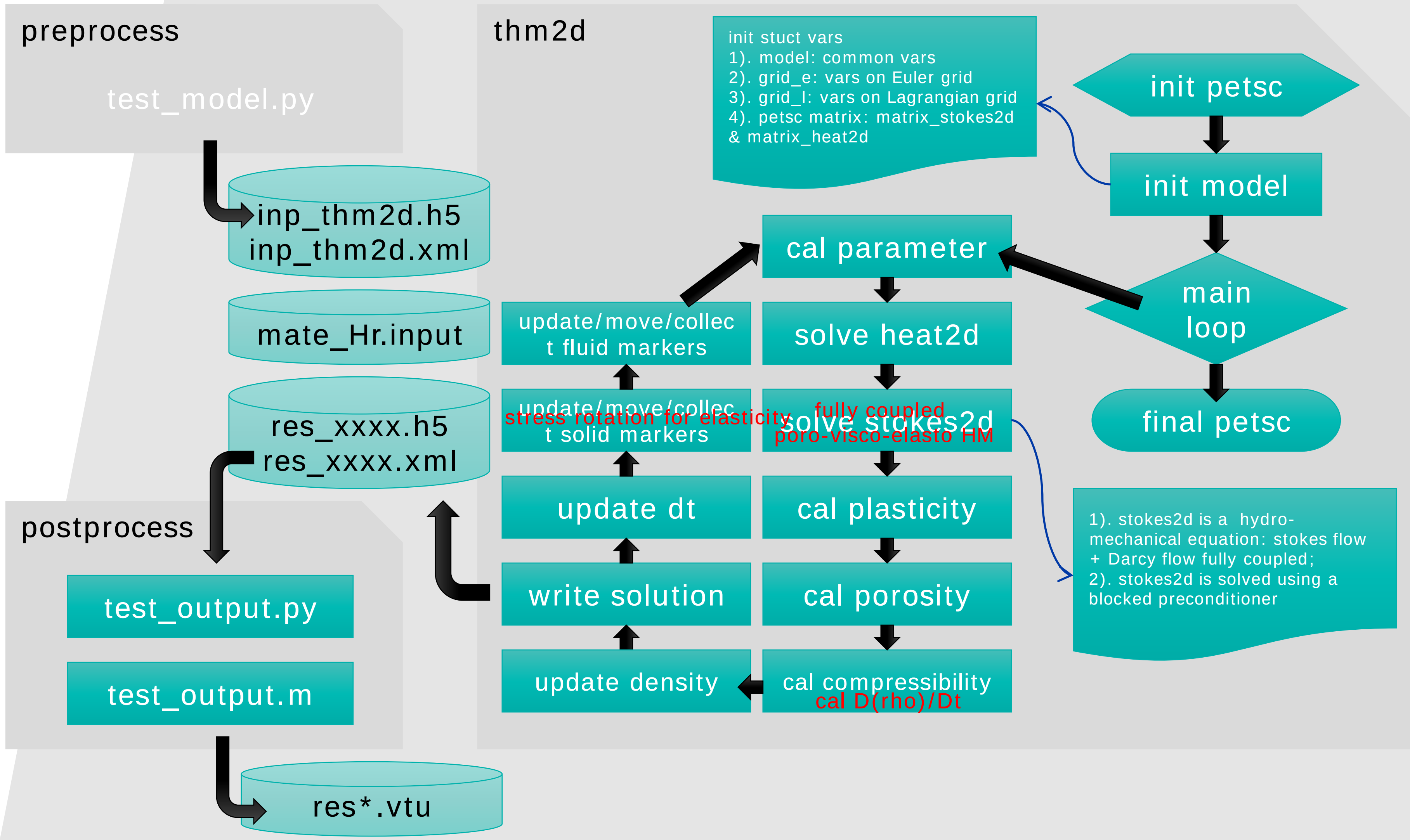
$$\zeta = \eta/\phi$$

$$\mu = \mu_0\left(1 - \frac{\phi}{\phi_c}\right)$$

Numerical Implementation
Design & Principles

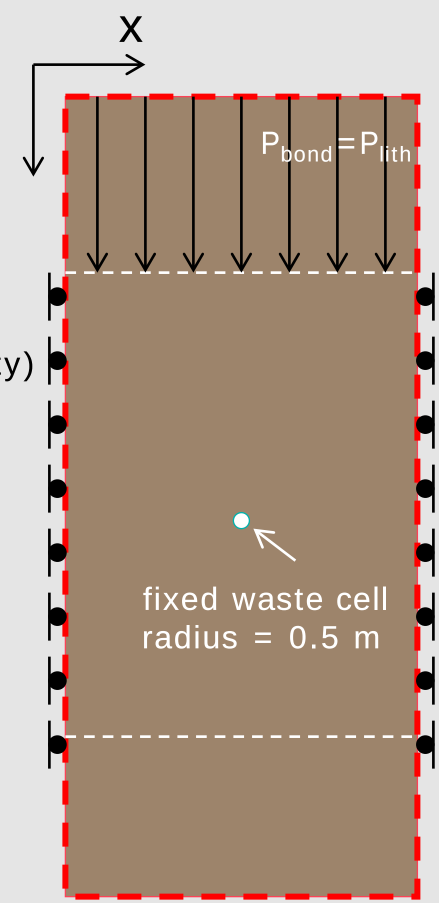
- Same principles as Geodynamics code: Finite Differences with staggered grid and moving marker technique
- 2 dimensional
- C code, python & matlab scripts support for interface, hdf5 & XML2 I/O data
- support vtk format for visualization
- PETSc based blocked preconditioned solver. The developed code is massively parallel

Numerical Implementation
Flowchart



Test 2D Simulation - Setup

- The test calculation represents a cross section of a HLW cell in a clay host rock
- 200m x 60m; waste cell at the center
  - Typical thickness of host rock, typical spacing between HLW cells
- Parameters from literature:
  - Opalinus clay / Callovo-Oxfordian clay when available
  - Other rocks or extrapolations when not available (shear viscosity)



Host rock (clay rock):

ρ = 2500 kg/m³
η_{bulk} = 1.0E18 Pa.s η_{fluid} = 1.0E-3 Pa.s
μ = 1.0E10 Pa (shear modulus)
Cp = 860 J/Kg/K
kx = 2.1, ky = 1.2 W/m/K
(anisotropic thermal conductivity)
α = 2.0E-5 1/K (thermal expansion)
K = 1.0E-13 m/s (hydraulic conductivity)
ϕ = 0.11 (initial porosity)

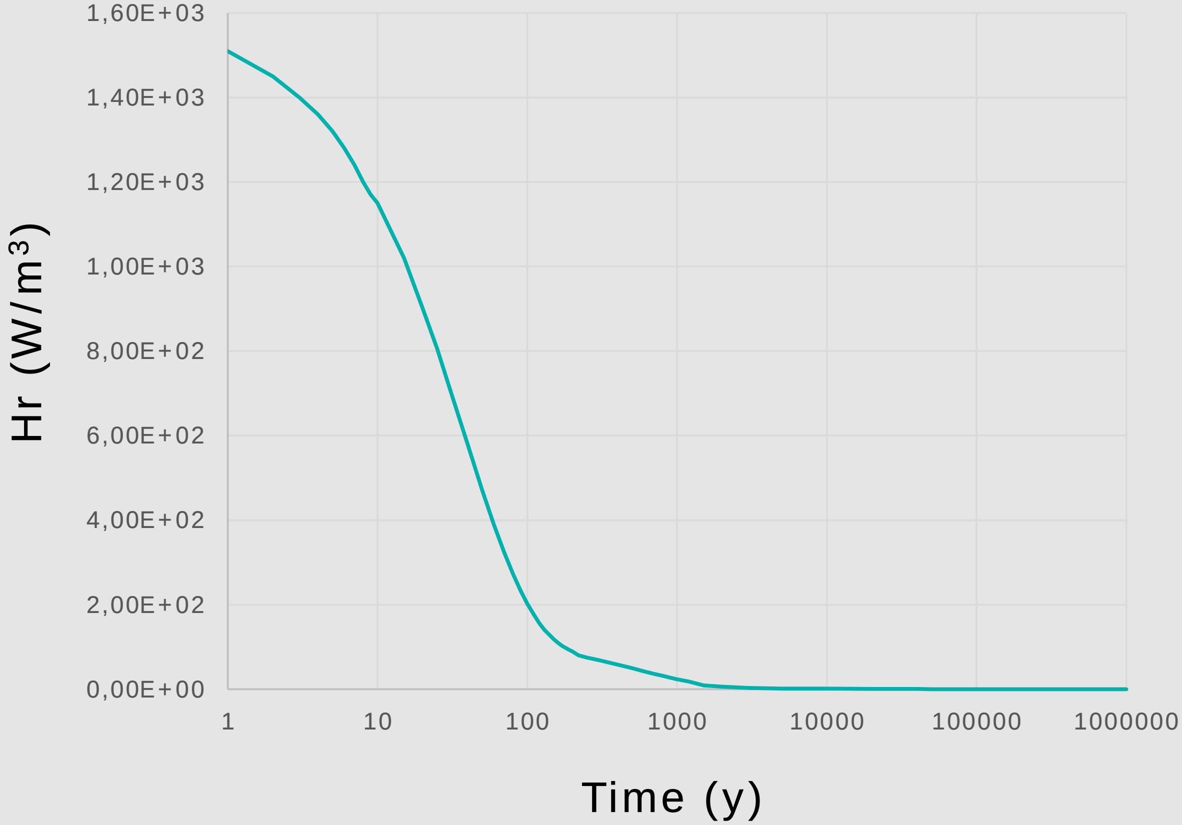
Waste cell

ρ = 3500 kg/m³
η_{bulk} = 1.0E20 Pa.s
Cp = 900 J/Kg/K
kx = 0.6, ky = 0.6 W/m/K
K = 1.0E-6 m/s
(hydraulic conductivity)

η_{fluid} = 1.0E-3 Pa.s
Initial Temperature:
geothermal gradient

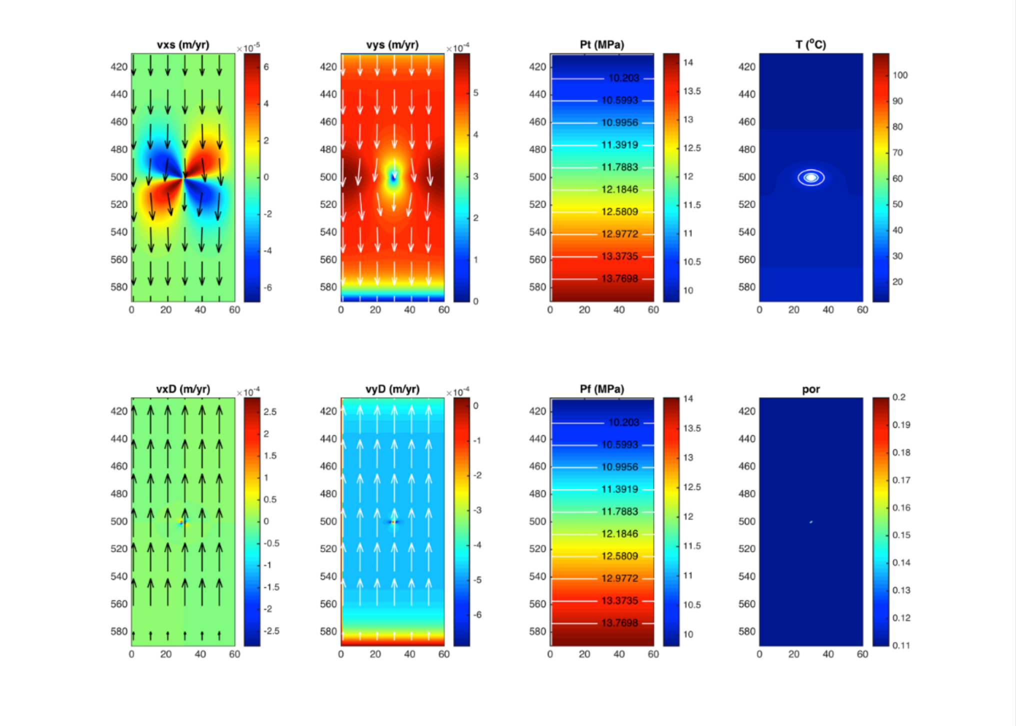
Test 2D Simulation - Setup

- Heat source term typical of HLW



Test 2D Simulation - Results

- At waste emplacement time: 0 yr
- no compressibility, thermal expansion, plasticity effects
- Compaction dominates



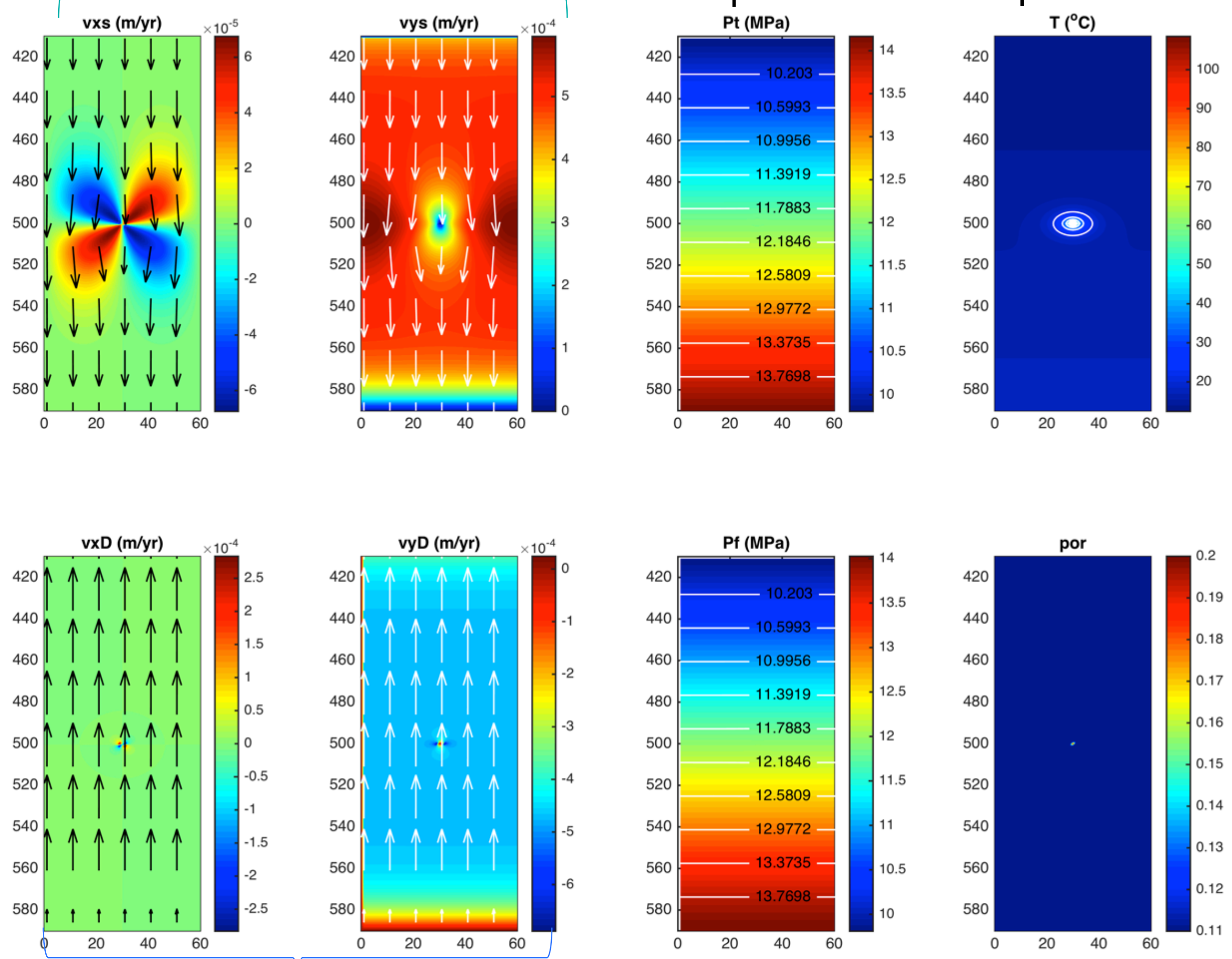
Test 2D Simulation - Results

Bulk displacement velocity: x & y components + vector

Total pressure

Temperature

(t = 0 year)

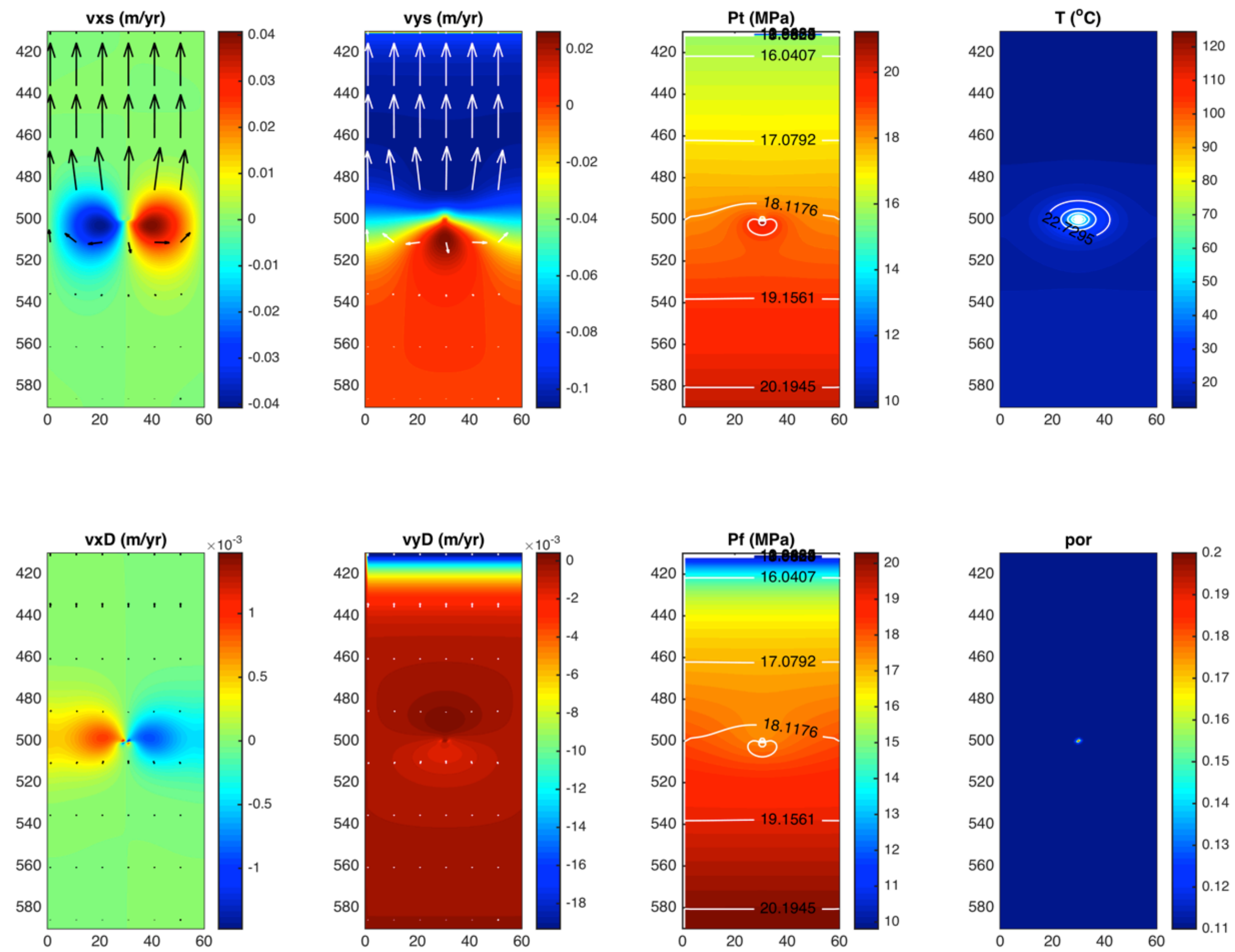


Darcy velocity: x & y components + vector

Fluid pressure

Porosity value

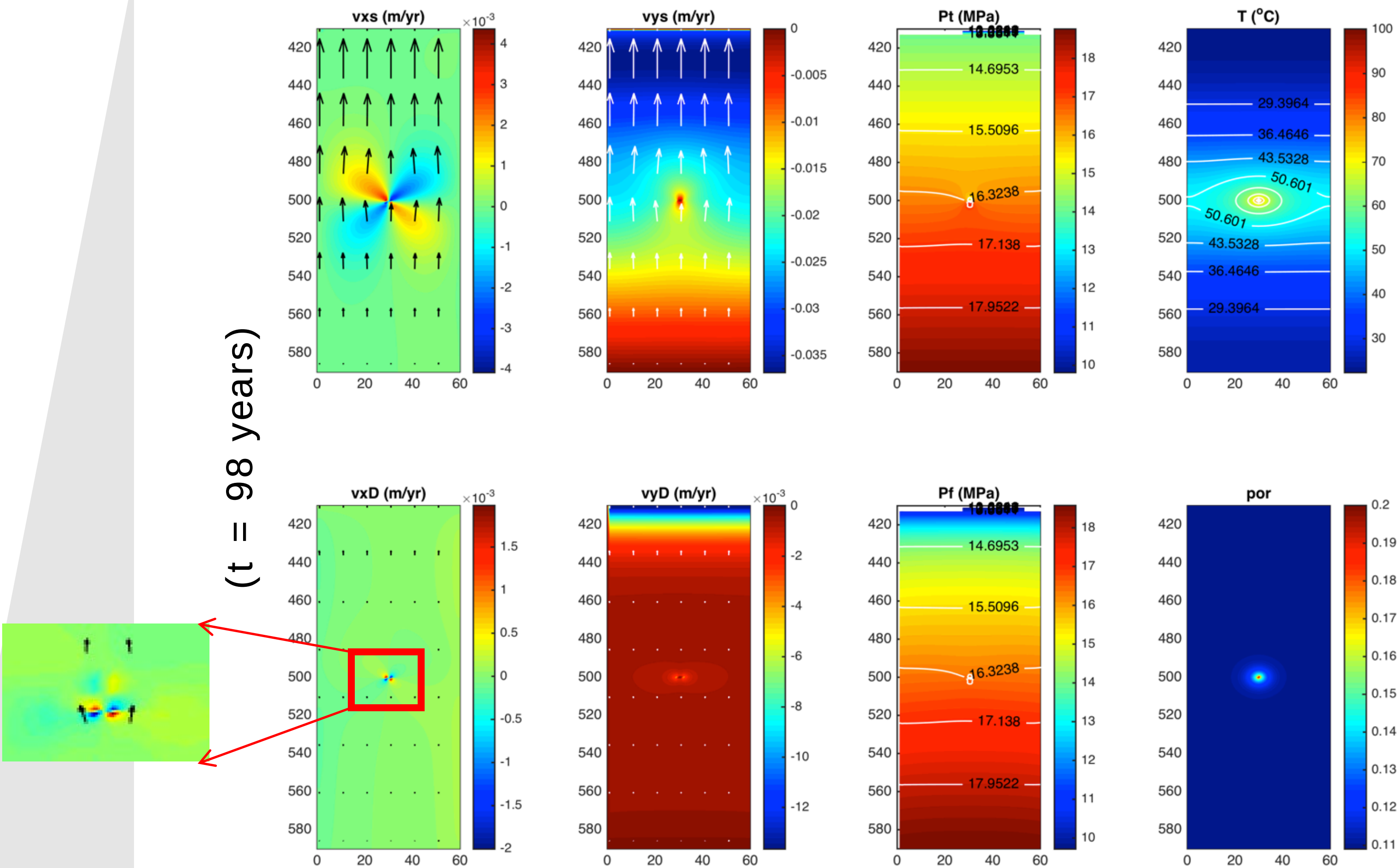
Test 2D Simulation - Results



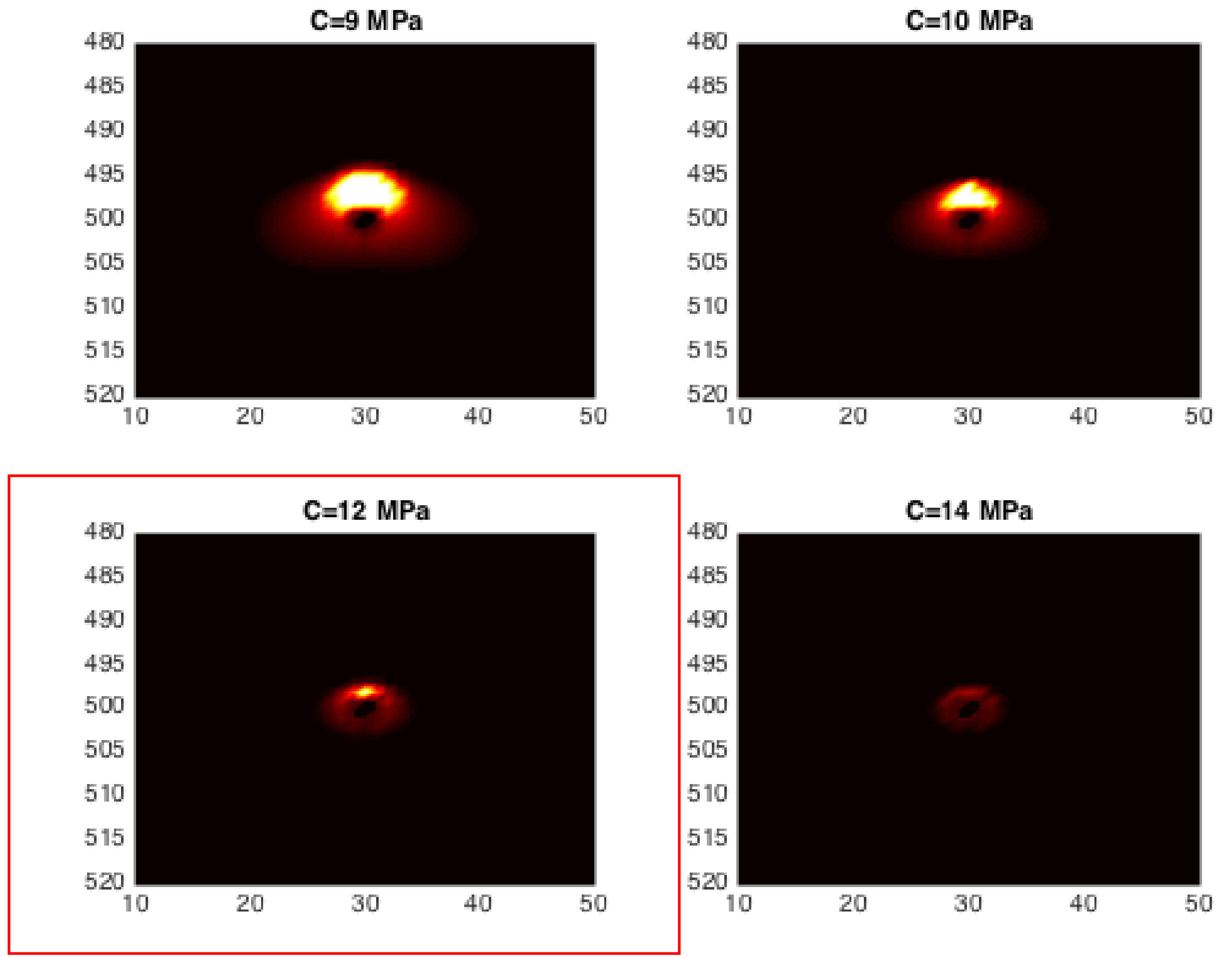
(t = 2 years)

Test 2D Simulation - Results

(t = 98 years)



Test 2D Simulation - Results



Identified micro fracturing zones for different cohesion values (9-14 MPa)

Test 2D Simulation - Results

- At waste emplacement time: 2 years and 98 years
- Host rock heats up:
  - highest value next to waste: ~100°C, ~50°C in near field (corresponding to typical HLW dimensioning values)
- THM effects:
  - Expansion of fluid and skeleton
  - “Swelled” rock with upwards displacement where thermal impact (2yr vs. 98 yr)
  - Water squeezed upwards too; higher v than before heating (beware of scale!)
  - Porosity changes (increase) next to the waste cell

Conclusions

- A 2D THM code adapted from plate tectonics was developed

with visco-elasto-plastic behaviour including compressibility of fluid & solid and thermal coupling

- It was able to compute a reality-inspired case and show:
  - Coupled THM effects
  - Skeleton expansion and displacements of rock and squeezed water
  - Micro-fracturing patterns at the vicinity of the waste cell

  The obtained value ranges appear reasonable

- The convergence of the algorithm was very good (CPU times of few minutes on ~300 000 cells grid with 1 year time steps)
- This numerical experiment, as a proof of concept, shows the potential of this fully implicit scheme for modeling THM phenomena in and around a radioactive waste repository

Next Steps

- **Work on a more realistic case:**
- Improve initial/boundary conditions ...
- Improve parameter definition and parameter dependencies
  - Fluid viscosity function of temperature...
  - Values for clay (realistic shear viscosity, bulk compressibility, anisotropic permeability...)
  - Elastic compaction
- **Validation and benchmarking of the code**
- Relevant numerical test cases (large scale long term evolutions)
- Relevant laboratory and field experiments (heater experiments)
- **Improve numerical capacities**
- Multi-grid preconditioner for solid phase
- Improve parallel resolution and support 3D models
- Adaptive mesh refinement