Modelling Geological Nuclear Waste Disposal : Some Thermo-Hydro-Mechanical (THM) problems in porous media

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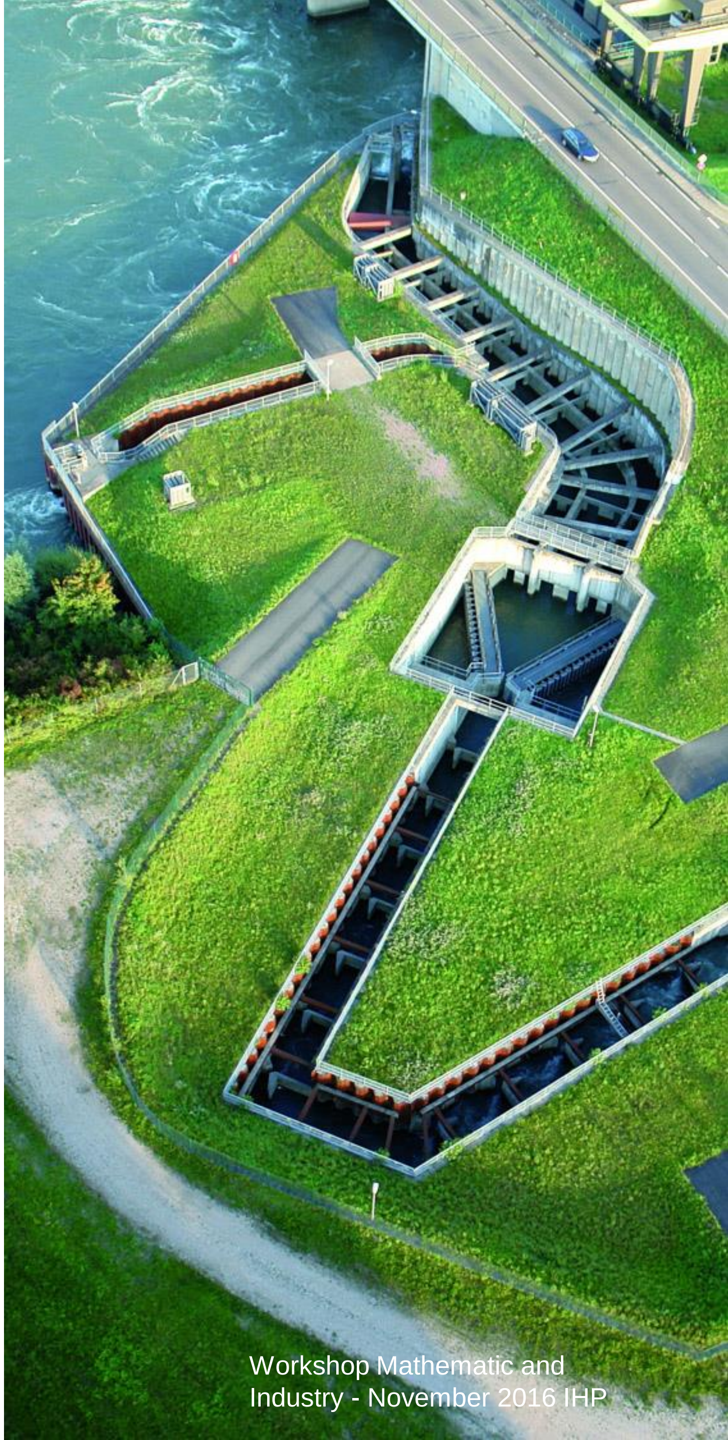
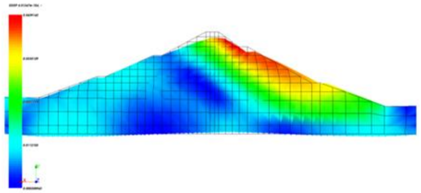
Outline

- General Context
- General Macroscopic THM model description
- Examples of THM problems
  - ✓ Mechanical laws and numerical treatments
  - ✓ Simulation of in situ experiment
- Numerical locks and perspectives
- General Conclusions

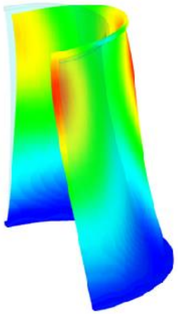


General Context (1/4)

Multiphysic problems in porous media in electricity industry

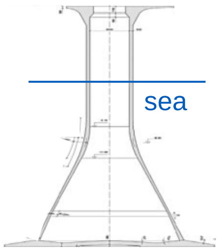


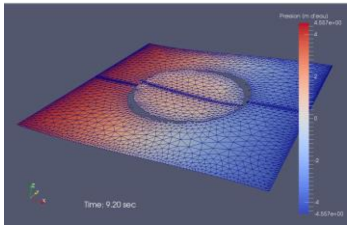
- Hydraulic buildings (dams …)
  - Coupling between hydraulic and mechanic (impoundment, emptying, level variation)
  - Seismic risk (dynamic problems)



- Containment structures, air coolers
  - Coupling between H, T, and M
  - Estimation of leakage in concrete structures

- Wind turbine
  - Modeling of the ground (flow, overpressure, hydrodynamic loading …) under a Gravitary Based Structure (BGS)



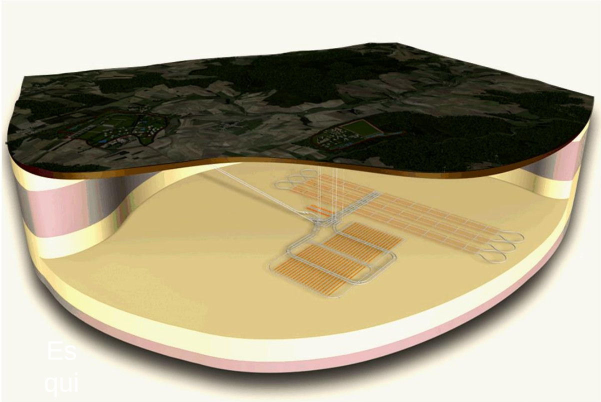


Water Pressure (Flejou 2016)

General Context (2/4)

Nuclear waste disposal (responsible : Andra)

- A network of galleries and cells in Callovo-Oxfordian argillite (- 500 m)

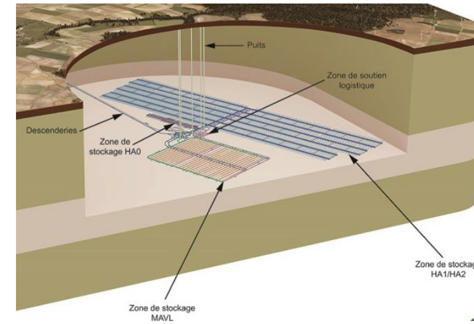


Esquisse Andra

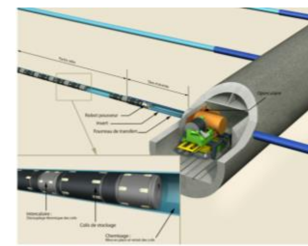
- Robustness and safety
- Dimensioning and optimization of the geometry (compactness of the installations)

General Context (3/4)

Issues for porous media modeling in nuclear waste disposal



- Near Field THM modeling
  - Estimation of the Excavation Damage Zone (EDZ) around galleries and cells – Study of the digging
  - Study of the concrete –> dimensioning of concrete lining
  - Understanding and prediction of the comportment of sealings and plugs : swelling and saturation/desaturation mechanisms
  - Comportment of voids between materials
  - Estimation of temperature and liquid pressure due to thermal dilatation – Mechanical consequences
  - Estimation of the Hydrogen pressure (corrosion, radiolysis) and Gas preferential pathways



Esquisse Andra

- Package modeling
  - Radiolysis Hydrogen production in cementitious package (surface disposal)
  - Bituminous package : risk of swelling under water uptake => THMC problem (multicomponents)

General Context (4/4)

- Specificities
  - A fully coupled T.H.M (C) problem (Multiphysic problem)
  - A complex geometry : 3D, from cells to geological layer ; crossing of galleries
  - Time dependant problem at different scales from tunnel excavation until post-closure stage : evolution of excavation, creeping of host rock, thermal problem, hydrogen production …
  - Heterogeneous materials with high contrasts and specific comportments
    - Intact or damage host rocks, sealing, plugs, concrete, bituminous, steels …
    - Goal of anisotropy
  - High contrast of initial conditions: stiff front
  - Hydraulic specificities : low permeability, weak desaturation of host rock, high level of capillary pressure and of water and gas pressure …

=> Software Code_Aster (www.code_aster.org)

High number of parameters and high number of experimental data =>
Uncertainties management becomes a crucial issue

Basic THM model

- Hypothesis of a classical model (Coussy formulation)
  - Anisotropic porous media constituted by 3 phases (compressible liquid + gas + solid) and 2 components (ex. H_20 and H_2)
  - Equilibrium equations
    - Mass conservation of each component (classical two-phase flow model)

$$\dot{m}_l^c + \dot{m}_g^c = div(\mathbf{F_l^c} + \mathbf{F}_g^{\mathbf{c}}) = 0 \quad c = H_2, w$$

    - Mechanical equilibrium (total stresses)

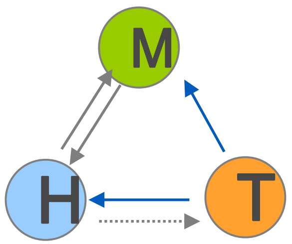
$$\mathbf{Div}(\sigma) + r\mathbf{F^m} = 0$$

    - Energy conservation
  - Component laws
    - Darcy law on each phase (liquid and gas) $\dfrac{\mathbf{F_p}}{\rho_p} = \dfrac{\mathbf{K^{int}}.k_p^{rel}(S_p)}{\mu_p}\left(-\nabla p_p + \rho_p \mathbf{g}\right) \quad p = l, g$
    - Porosity evolution linked to solid deformation and dilatation
    - Diffusion : Fick's law for each mixture
    - Gas perfect law
    - Dissolution : Henry's law
    - Vaporization
    - Mechanical laws : $\boldsymbol{\sigma}' = f\left(\varepsilon, \ldots\right)$ several comportment laws adapted to each material (elastic, elastoplastic, viscoplastic, thermo-viscoplastic …)

T.H.M couplings description

Mechanic -> Hydraulic

✓Fully saturated medium : Biot relation

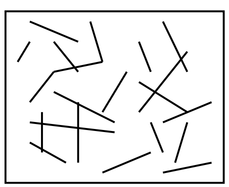


$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' - b p_l \mathbf{I}$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' - b\left(S_l\, p_l + S_g\, p_g\right)\mathbf{I}$$

Hydraulic -> Mechanic

✓Permeability affected by damage



homogenisation → Damage ↔ K

Ex.: $K(\varphi) = f\left(k_0.(\varphi - \varphi_0)^3\right)$

✓Thermic =>Hydraulic : Dilatation of water

✓Thermic=>Mechanic : Dilatation of skeleton and mechanical stresses due to temperature

✓Hydraulic=> Thermic: effect of desaturation

General numerical choices

- Fully Coupled formulation T,P,U
  - ✓ Two-phase flow modeling : unknowns adapted to gas appearance/desappearance treatment (Angelini et al. 2010)

$$(P_l, \chi_l^{H_2} = \frac{K_H \rho_l^{H_2}}{M^{H_2}}) \text{ instead of } (P_l, P_g)$$

- Finite Elements P2P1 (2D, AXI, 3D) or VF SUSHI for pure hydraulic problems (Angelini et al. 2010)

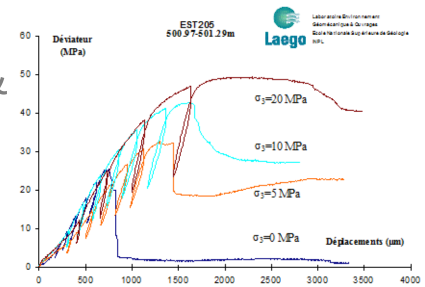
- Time Euler implicit

- High non linear (S(Pc), kr(S)…) problem solved by Newton Method + Linear research (Newton Krylov available)

- Linear problems solved by direct methods (Mumps) or iterative methods (from PESTC : BCGS, GMRES, etc.)

Mechanical laws and treatment (1/4)

- Mechanical law adapted to material rheology :
  - For Callovo Oxfordien argilite (ex. L&K, Hoek & Brown…):
    - •Brittle behavior of the rock
    - •Softening behavior
    - •Dilatancy
    - •Creeping phenomena (viscoplasticity)



Risk : apparition of localization effects due to strong micro deformation gradient not included in classical treatment (only on macroscopic variables)

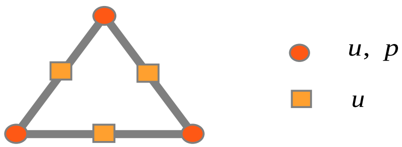
➡ Results are dependent of grid !

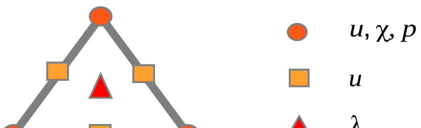
Methods of regularization : non local model using a microscopic field

=>Micro Gradient Dilation Model (Fernandes et al. 2009) – regularization only on volumic strain (second gradient)

$$\int_{\Omega}\left(\sigma_{ij}\varepsilon_{ij}^{*}+D.\frac{\partial \chi}{\partial x_j}\frac{\partial \chi^{*}}{\partial x_j}\right)d\Omega-\int_{\Omega}\lambda\left(\varepsilon_{V}^{*}-\chi^{*}\right)d\Omega=P_e^{*}$$

$$\int_{\Omega}\lambda^{*}\left(\varepsilon_{V}-\chi\right)d\Omega=0 \qquad \forall\,\lambda^{*}\in L^{ad}$$

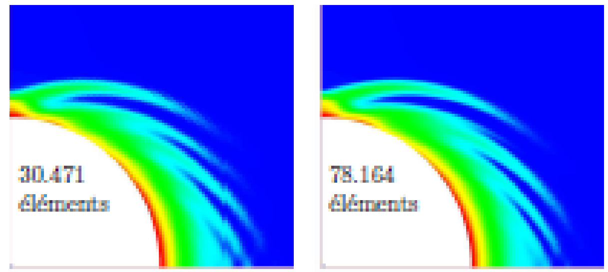




Mechanical laws and treatment (2/4)

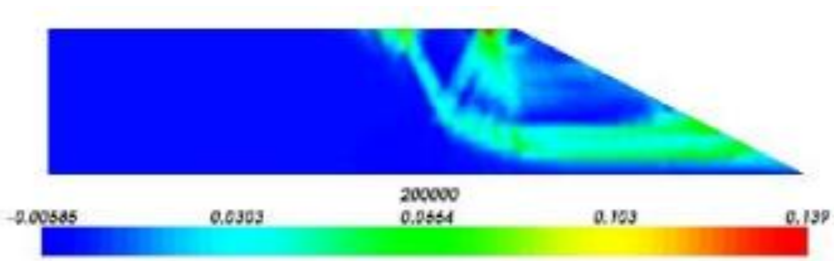
Porosity variation excavation problem without and with second gradient method (from MoMas Benchmark):

Without regularization

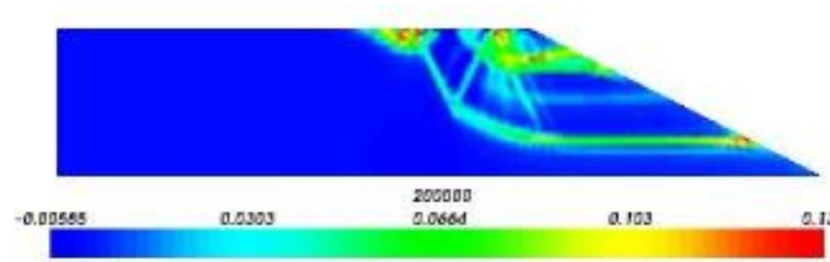


With 2d gradient

Plastic Volumic deformation in a dam modeling with 2d gradient (Foucault 2010) :



Coarse mesh



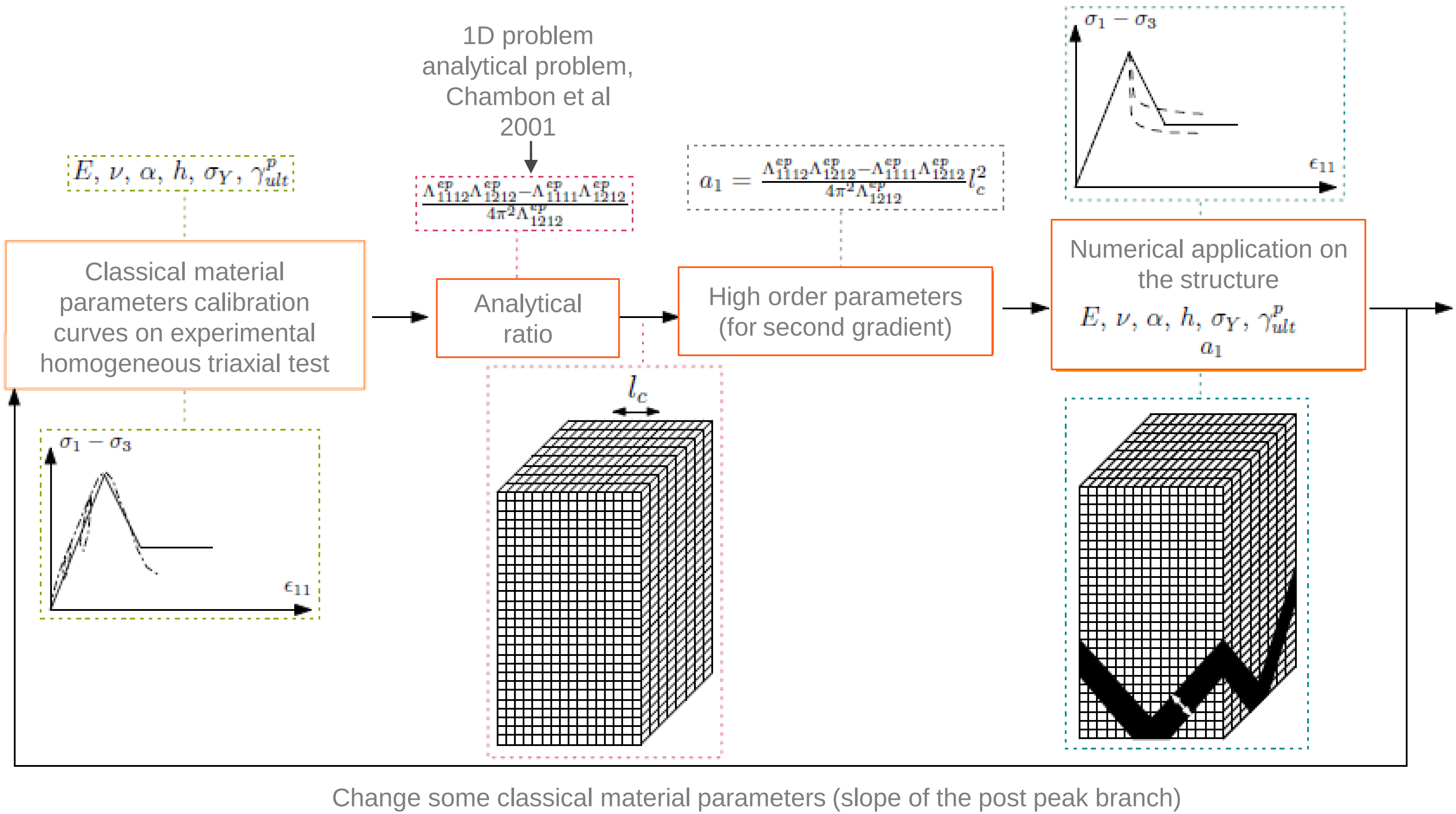
Fine mesh

Difficulty : Necessity of the introduction of additional parameters and internal length representative of localization pattern. A procedure is necessary

Mechanical laws and treatment (3/4)

Definition of a methodology to identify second gradient parameters (Raude et al. 2015 – collaboration with GeoRessources)

=>Combination of a triaxial test modeling and analytical 1D solution

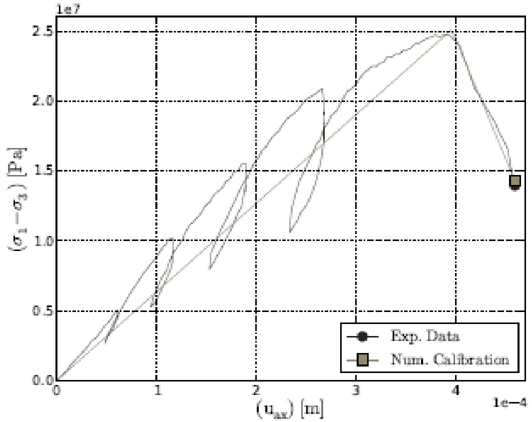


Mechanical laws and treatment (4/4)

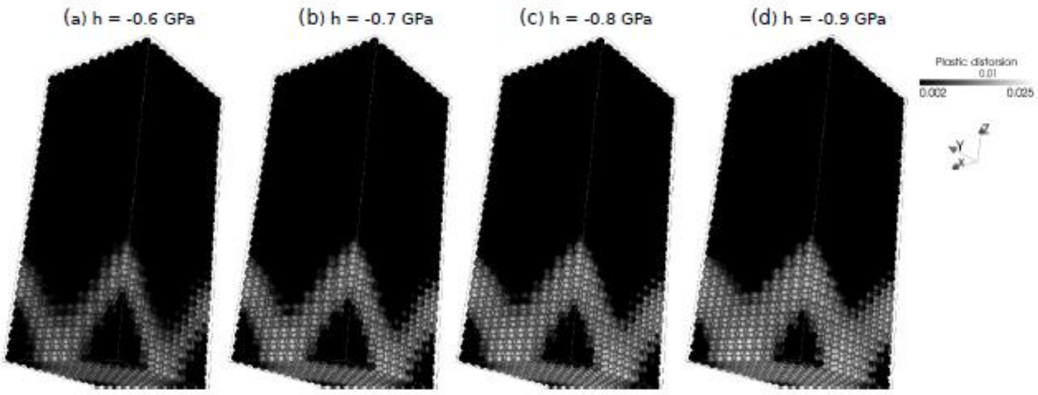
- Application to a shale specimen : Sisteron shale
  - Porous shale specimens from Sisteron : triaxial tests (GeoRessources)
  - Elasto-plastic law : Drücker Prager

=>First hypothesis : we consider that characteristic length is about 1/3 of the horizontal size of the specimen

First step : Calibration of the Drücker Prager parameters



Distribution of the accumulated plastic shear for different slopes for a fixed lc



- Same results obtained with different meshes
- Perspective : Generalization of this method on different rocks and complex laws

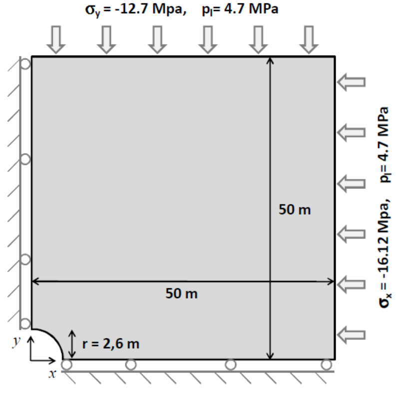
Mechanical Numerical simulations (1/3)

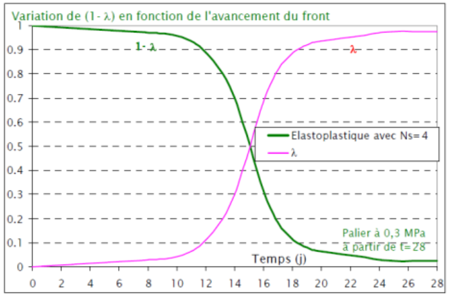
Context : Andra numerical benchmark exercise (Cuvilliez et al. 2014)

- Goal : compare numerical results of underground excavation to experimental measures (based on a realistic experiment of tunnel digging in Bure)
- Evaluate effect of HM couplings, concrete lining, etc.
- Data : geometry, advancement of digging, etc.

Computation hypothesis :

- 2D modeling using convergence-confinement method



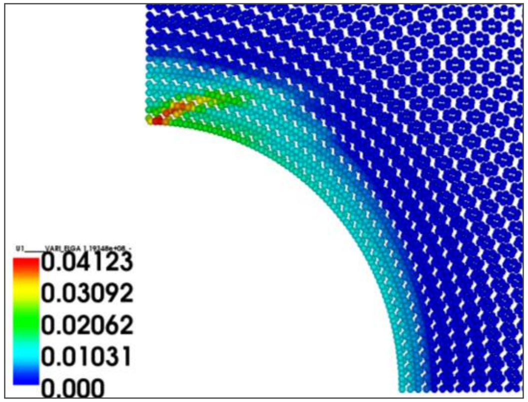


- Mechanical law : specific elasto-visco-plastic law (Laigle & Kleine)
- Coupling with hydraulic (HM simulation)
- Using of a regularization model

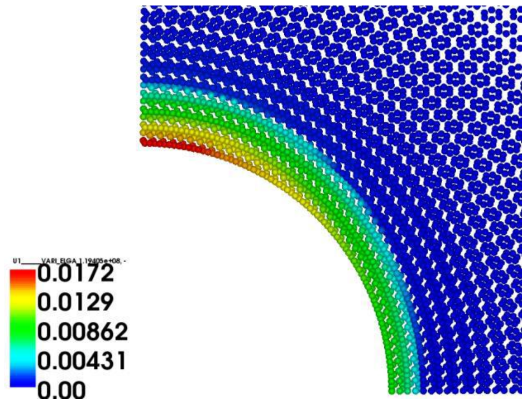
Mechanical Numerical simulations (2/3)

- Goal of regularization

Plastic strain hardening

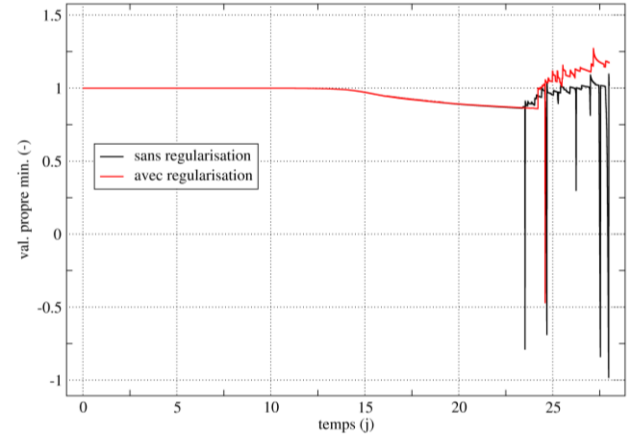


Local modeling

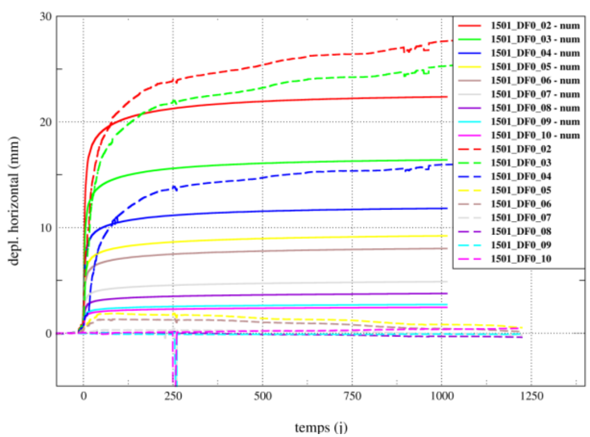


With regularization

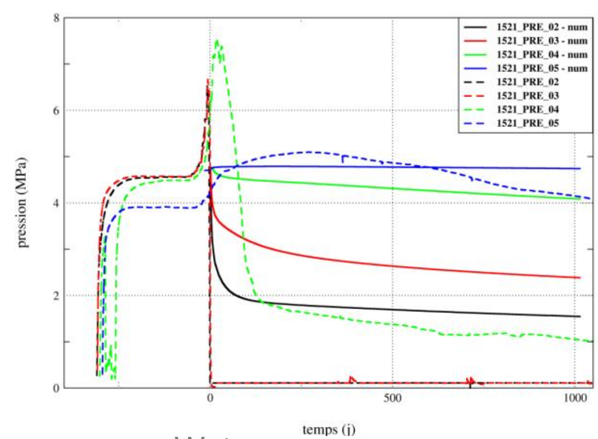
Eigenvalue evolution in Jacobian Matrix



- Comparison with experimental results



Vertical displacement



Water pressure

Mechanical Numerical simulations (3/3)

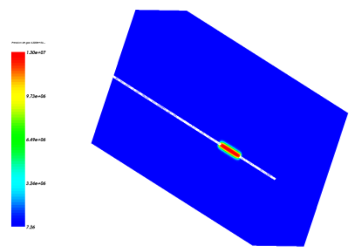
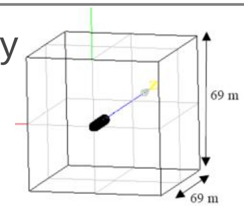
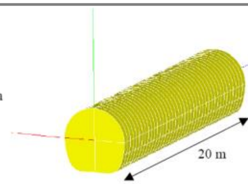
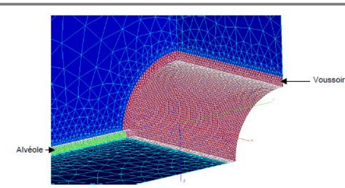
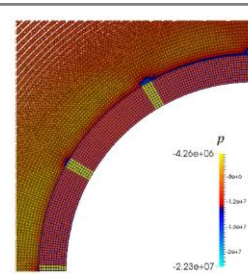
Conclusion of Andra Benchmark simulation

- Numerical predictions are consistent with experimental results: water pressure drop and displacement well reproduced
- Necessity to have a coupling HM modeling even for displacement reproduction
- Necessity of non local method to avoid mesh dependency

- In the future 3D modeling will be necessary to reproduce correctly digging advancement (convergence confinement method is limited)

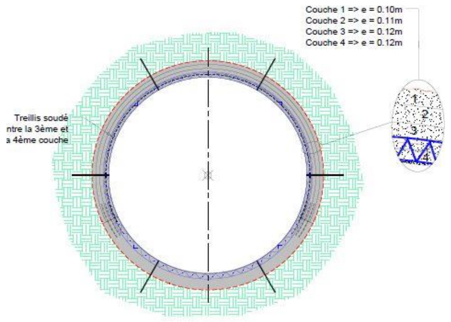
➡ More complexity is required

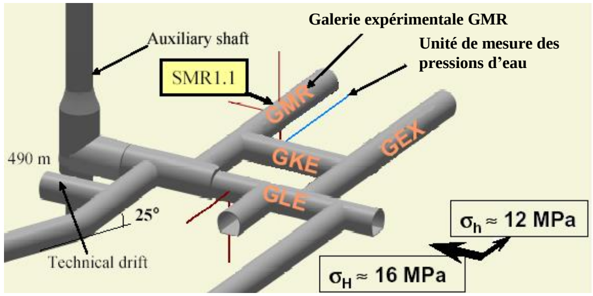
What we can do (overview)

Geometry (example)	Mechanisms
Ex : PGZ1 experiment modeling (FORGE Project) Injection of Hydrogen in anisotropic initially saturated host rock (Granet et al, 2010) 	HM (elastic) – two phase flow – several materials 3D ≈ 1 Millions DOF
Ex : Modeling of GMR Gallery (Meunier et al., 2011)  	HM (elastic)– realistic modeling of digging One material 3D ≈ 3 Millions DOF
Ex : 3D Modeling of High Activity cell 2015 	THM (viscoplastic law)– homogeneous digging 3D– 2d gradient ≈ 1 Millions DOF
Ex : 2D Modeling of a Gallery digging and concrete installation with compressible wedge and interface 	THM (viscoplastic) – 2d gradient – Simple modeling of digging (convergence confinement) – numerous heterogeneities 2D

What we would like to do in the future

- 3D Viscoplastic THM study with digging progression on a complex geometry (crossing of galleries)





Andra

- 3D two-phase flow THM problem with several materials on a complex geometry

  ➡ Today : too expensive, too long

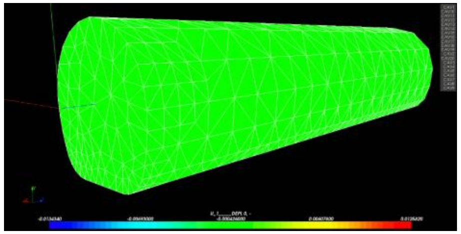
- More generally, we need :
  - More complexity (geometry, mechanisms, etc.) => more DOF and non linearities
  - More computations :
    - ✓ Sensitive analysis are required in order to reduce uncertainties
    - ✓ Experimental fitting

Numerical locks

- Very high non linear problems (mechanical laws, material parameters, etc.)

- Nature of the variables : multiple and heterogeneous
  - Convergence criterion difficult to define for Newton Method
  - Bad conditioning of Matrix =>Iterative solvers not optimized

- Time evolution of Interest area
- Mesh refinement criterion well adapted to Hydro-Mechanical problem not yet available => explosion of DOF



HM (elastic) study of a digging. Using Homard mesh refinement tool (Meunier et al 2011)

Numerical perspectives

- Better use of iterative solvers (HPC problems) adapted to parallelism

- PHD Thesis, Rita Riedlbeck, 2014-2017 (supervised by D. di Pietro and A. Ern)
  - ✓ Stopping criteria and adaptative schemes for non linear Hydro-Mechanical problem (poroelasticity and poroplasticity)
  - ✓ Extension to poromechanical problem of a posteriori error estimates by equilibrated reconstructions of velocity and stress (Ern et Vohralik 2010). Flux equilibrium allows a systematic normalization.
  - ✓ Dominant error criterion for linear solvers
  - ✓ Dynamic adaptation of time and space step

Cf. Talk of Rita Riedlbeck tomorrow !

Conclusions and general perspectives

- **A Fully T.H.M tool with several possibilities in Code_Aster**
  - More and more complexity : complex 3D structural problems, phenomena to take into account … => HPC problems
  - More and more sensitive computations are required in order to improve waste disposal dimensioning and robustness
  - New model (Chemico-Hydro-Mechanical problems for bitumen swelling modeling – PHD thesis of G. Melot)

- **Link with experimental tests is crucial**
  - Calibration of numerical tools (ex : characteristic length)
  - Calibration of data
  - More and more comparisons with experiments are required
  - How to deal with dispersion of experimental data ? => uncertainties management will be a crucial issue