Università degli Studi di Padova

Multiphysics modelling of thermal cracks in multiphase heterogenous porous materials

Zechao Chen -- 38th cycle

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Co-supervisor: Prof. Laura De Lorenzis, ETH Zurich

PhD Course in Sciences, Technologies And Measurements For Space

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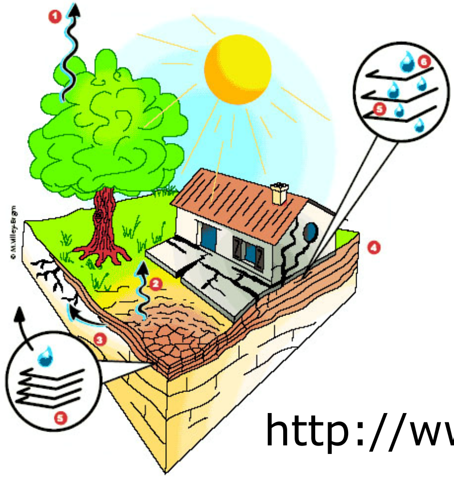
Motivation: cracks due to hydro-thermal effects

Desiccation (Laloui 2009)



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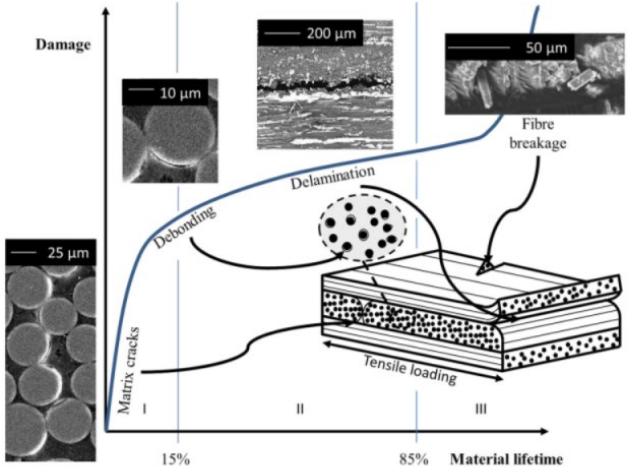
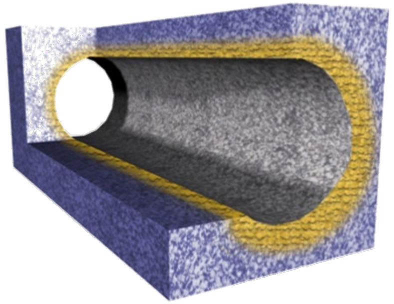
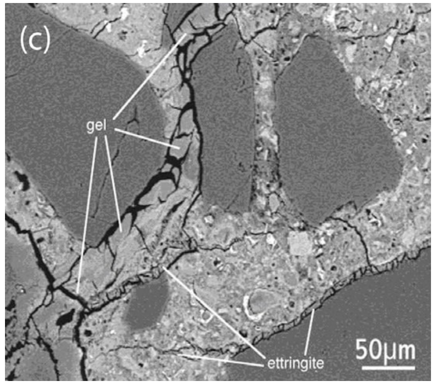


Damage in composite laminates doi.org/10.1007/s10853-018-2045-6

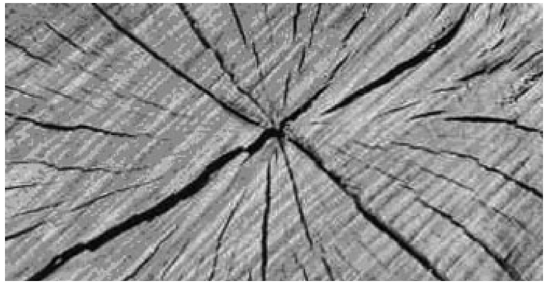
Desaturation/cracks developement of EDZ (Excavation Damaged Zone)

Deep nuclear waste disposals





ASR (Alkali-Silica Reaction) shrinkage-induced cracking in concrete



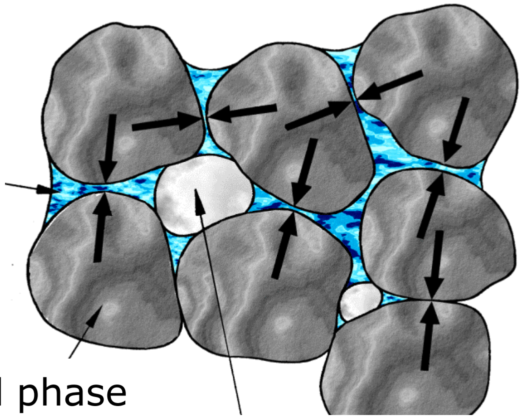
Cracks in wood

2. Research background

Multi-phase porous material

Composed by a solid skeleton with open pores containing one or more fluids

liquid phase: water

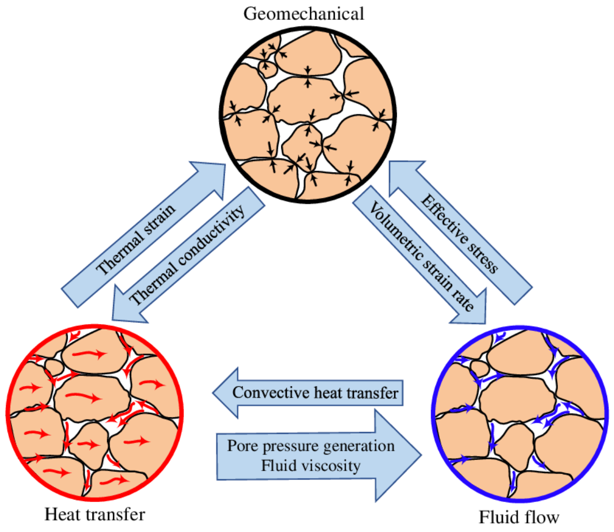


Microscopic view of a three-phase material

Intergranular forces due to capillary effects

solid phase

gas phase: dry air and water vapour



Mechanics of multi-phase porous materials

solid-fluids interaction, liquid-gas interaction, non-isothermal conditions

- *Lewis, R. W., Schrefler, B. A. 1998. The Finite Element Method in the Static and Dynamic Deformation and Consolidation of Porous Media (Second.). Chichester, UK: John Wiley & Sons.*
- *William G. Gray, Cass T. Miller 2014. Introduction to the Thermodynamically Constrained Averaging Theory for Porous Medium Systems. Springer.*

2. Research background

Multi-phase porous material

Equilibrium equations (mixture; quasi-statics):

$$div\left(\boldsymbol{\sigma}'-\left[p^g - S_w p^c\right]\mathbf{1}\right)+\rho\mathbf{g}=0$$

Mass balance equation (solid, liquid water and water vapour):

$$n\left[\rho^w-\rho^{gw}\right]\left[\frac{\partial S_w}{\partial t}\right]+\left[\rho^w S_w-\rho^{gw}\left[1-S_w\right]\right]div\left(\frac{\partial \mathbf{u}}{\partial t}\right)+\left[1-S_w\right]n\left[\frac{\partial \rho^{gw}}{\partial t}\right]$$
$$-div\left(\rho^g\frac{M_a M_w}{M_g^2}\mathbf{D}_g^{gw}grad\left(\frac{\partial p^{gw}}{\partial p^g}\right)\right)+div\left(\rho^w\frac{\mathbf{k}k^{rw}}{\mu^w}\left[-grad(p^g)+grad(p^c)+\rho^w\mathbf{g}\right]\right)$$
$$+div\left(\rho^{gw}\frac{\mathbf{k}k^{rg}}{\mu^g}\left[-grad(p^g)+\rho^g\mathbf{g}\right]\right)-\beta_{swg}\frac{\partial T}{\partial t}=0$$

Dry air mass balance equation:

$$-n\rho^{ga}\left[\frac{\partial S_w}{\partial t}\right]+\rho^{ga}\left[1-S_w\right]div\left(\frac{\partial \mathbf{u}}{\partial t}\right)+nS_g\frac{\partial \rho^{ga}}{\partial t}-div\left(\rho^g\frac{M_a M_w}{M_g^2}\mathbf{D}_g^{ga}grad\left(\frac{p^{ga}}{p^g}\right)\right)$$
$$+div\left(\rho^{ga}\frac{\mathbf{k}k^{rg}}{\mu^g}\left[-grad(p^g)+\rho^g\mathbf{g}\right]\right)-\left[1-n\right]\beta_{swg}\rho^{ga}\left[1-S_w\right]\frac{\partial T}{\partial t}=0$$

Energy balance equation (mixture):

$$\left(\rho C_p\right)_{eff}\frac{\partial T}{\partial t}+\rho^w C_p^w\left(\frac{\mathbf{k}k^{rw}}{\mu^w}\left[-grad(p^g)+grad(p^c)+\rho^w\mathbf{g}\right]\right)\cdot grad(T)$$
$$+\rho^g C_p^g\left(\frac{\mathbf{k}k^{rg}}{\mu^g}\left[-grad(p^g)+\rho^g\mathbf{g}\right]\right)\cdot grad(T)-div\left(\chi_{eff}\,grad(T)\right)=-\dot{m}_{vap}\,\Delta H_{vap}$$

- *Lewis, R. W., Schrefler, B. A. 1998. The Finite Element Method in the Static and Dynamic Deformation and Consolidation of Porous Media (Second.). Chichester, UK: John Wiley & Sons.*

2. Research background

The Phase-Field Method (PFM) to fracture

Energy functional

elastic strain energy — fracture energy

$$\min_{\mathbf{u}\in\mathcal{U}_n, d\geq d_{n-1}} \mathcal{E}_\ell(\mathbf{u}, d) = \int_\Omega [g(d)\boldsymbol{\psi}^+(\varepsilon(\mathbf{u})) + \boldsymbol{\psi}^-(\varepsilon(\mathbf{u}))]d\Omega + \frac{G_c}{c_w}\int_\Omega \left[\frac{w(d)}{\ell} + \ell|\nabla d|^2\right] d\Omega - \int_\Omega \mathbf{b}_n \cdot \mathbf{u} d\Omega - \int_{\partial\Omega_N} \mathbf{t}_n \cdot \mathbf{u} dS$$

Amor et al. (2009)
Miehe et al.(2010) Freddi and Royer-Carfagni (2010)

Phase-field evolution equation $-2l\triangle d + \frac{1}{2l}d = \frac{2(1-d)}{G_c}\mathcal{H}$ $\mathcal{H}(\mathbf{x}, t) := \max_{\tau\epsilon[0,t]} \Psi^+(\varepsilon(\mathbf{x}, \tau))$

$g(d)$: degradation function

G_c : fracture toughness

ℓ: crack length scale parameter

$\mathbf{u}$: displacement field

d: crack phase-field

ψ: energy storage function (ψ^+ refers to tensile and deviatoric energy; ψ^- is compressive part)

:$w(d)$ local damage function

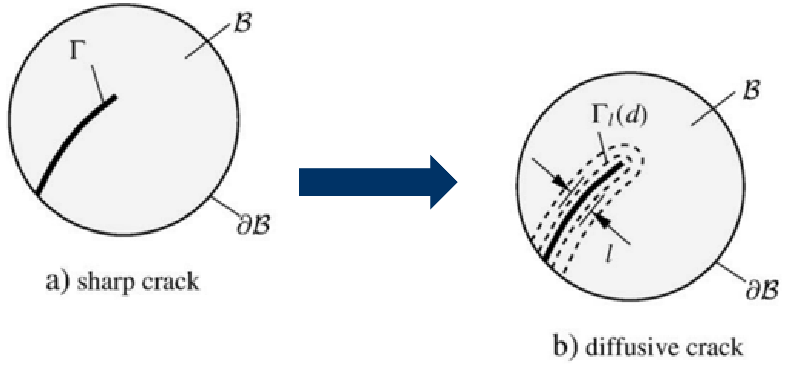
∇d: spatial gradient of d

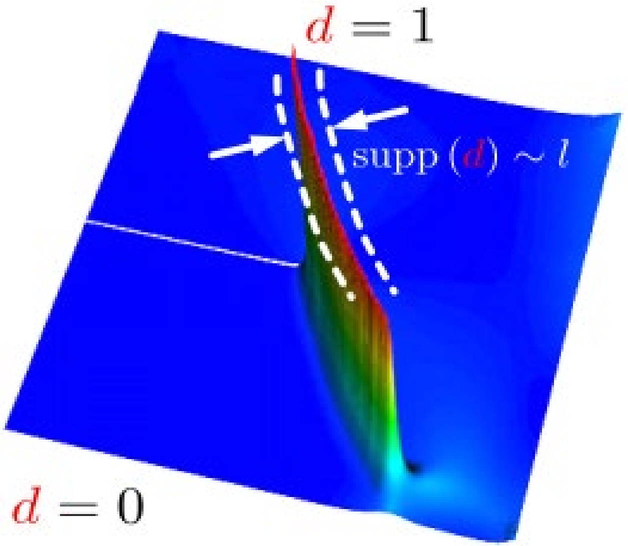
c_w: normalization constant

$\mathbf{b}_n$: body force vector $\mathbf{t}_n$: surface traction vector

2. Research background

The Phase-Field Method (PFM) to fracture





Key advantages

- Flexibility (initiation, propagation, merging, branching)
- Variational framework
- Simple implementation
- No ad-hoc criteria to model crack initiation and propagation

Disadvantages

- Fine mesh needed
- Efficiency/robustness of solution

- *SwissMech Seminars Archive – SwissMech Seminars*

3. Project objectives

1. Develop a *THM (Thermo-Hydro-Mechanical) crack Phase-field numerical model* able to study the nucleation and propagation of cracks induced by **thermal effects** in multiphase heterogenous porous materials.

merging a **thermodynamically consistent multiphase porous media model** (and the associated finite element code *Comes-Geo* developed at the UNIPD) with a **crack phase-field model** (and the associated *Griphfith* code for brittle fracture developed at ETH Zurich).

2. Application to study thermal shock cracks and desiccation cracks in clayey materials and in heterogeneous composite materials.
3. After **validation with experiments**, the model will be further **extended:**

   a) from quasi-statics to dynamics

   b) from brittle to ductile fracture

Algorithm implementation

Describing the coupled problem of poromechanics and cracking under thermal conditions in variably saturated porous media.

- Reference*: Cajuhi T, Sanavia L, De Lorenzis L. Phase-field modeling of fracture in variably saturated porous media[J]. Computational Mechanics, 2018, 61(3): 299-318.*

Initialization $(t = t_0 = 0)$**:** $\bar{\mathbf{u}}, \bar{\mathbf{t}}, \bar{p}, \bar{q}, \bar{d}, \mathcal{H} = 0$;
for $n = 0 : N\text{-}1$ **do**
  compute $\Psi^+(t = t_{n+1})$
  if $\Psi^+ > \mathcal{H}_n$ **then**
    $\mathcal{H}_{n+1} \leftarrow \Psi^+(t = t_{n+1})$;
  else
    $\mathcal{H}_{n+1} = \mathcal{H}_n$;
  end
  solve $d_{n+1}(\mathcal{H}_{n+1})$;
  solve $\mathbf{u}\text{-}p_w := \mathbf{U}_{n+1}(d_{n+1})$;
end

Algorithm 1: Algorithmic solution procedure for the $\mathbf{u}$-p_w-d system

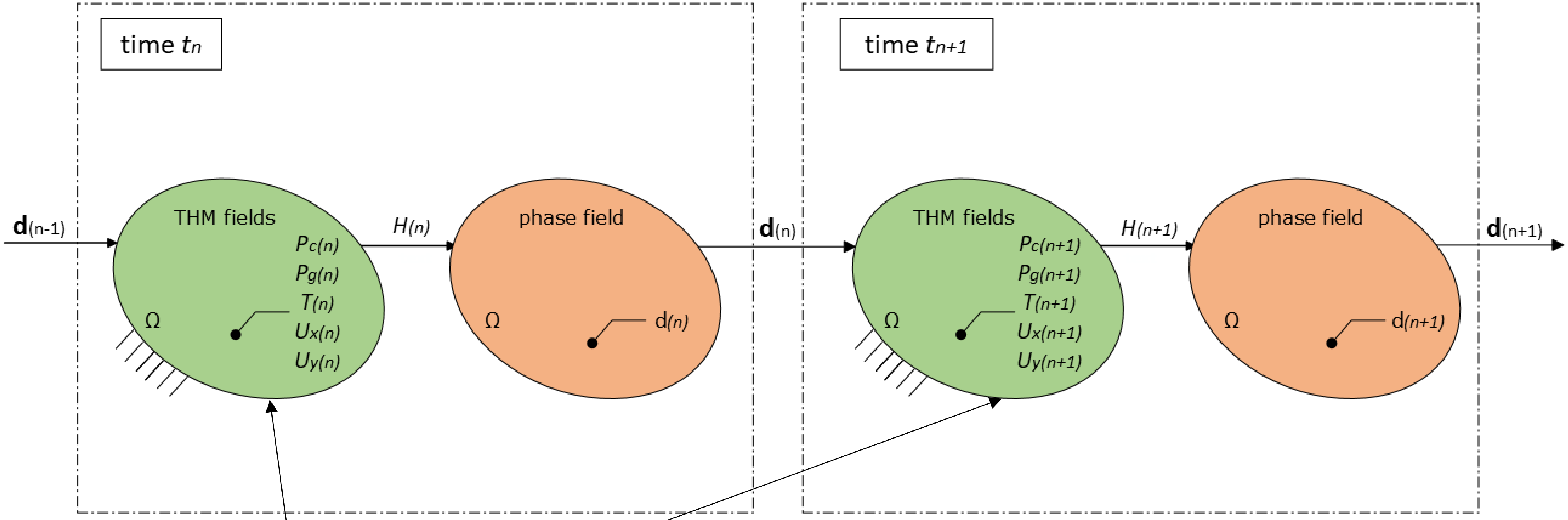
Previous algorithm

Initialization $(t = t_0 = 0)$: $\bar{\mathbf{u}}, \bar{\mathbf{t}}, \bar{p}, \bar{q}, \bar{d}, \mathcal{H}, \mathrm{T} = 0$;
for $n = 0 : N - 1$ *do*
  compute $\Psi^+(t = t_{n+1})$
  if $\Psi^+ > \mathcal{H}_n$ **then**
    $\mathcal{H}_{n+1} \leftarrow \Psi^+(t = t_{n+1})$;
  else
    $\mathcal{H}_{n+1} = \mathcal{H}_n$;
  end
  solve $d_{n+1}(\mathcal{H}_{n+1})$;
  solve $\mathrm{u} - p_c - p_g - \mathrm{T} := \mathbf{U}_{n+1}(d_{n+1})$;
end

Algorithm : Algorithmic solution procedure for the u-p_c-p_g-T-d system

New algorithm

Algorithm implementation

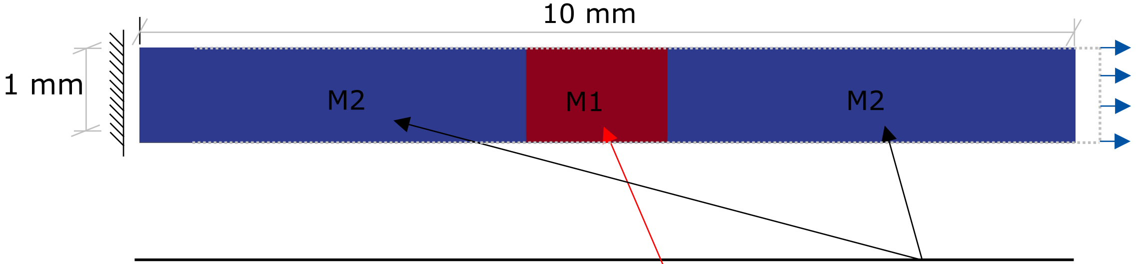


The illustration of solution procedure for five coupled fields.

The four THM equations are solved in a **monolithic** way; while the THM equations and phase field equation are solved with a **staggered** scheme.

Validation of the implementation: tensile test

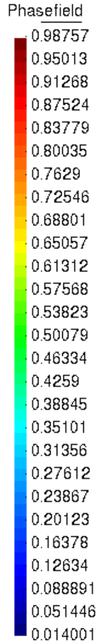
Pure Mechanical problem *with crack phase-field*



Material	M1	M2
Tensile strength (GPa)	**21**	**210**
Fracture Toughness-Gc (kN/mm)	0.0027	0.0027
Internal Length (mm)	0.4	0.4
Number of Elements	625	625

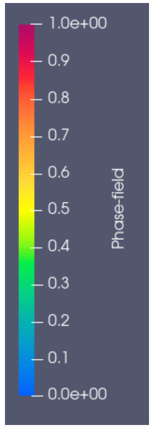
Tensile test of a bar, with a weaker material in the middle of the bar to trigger the cracking.

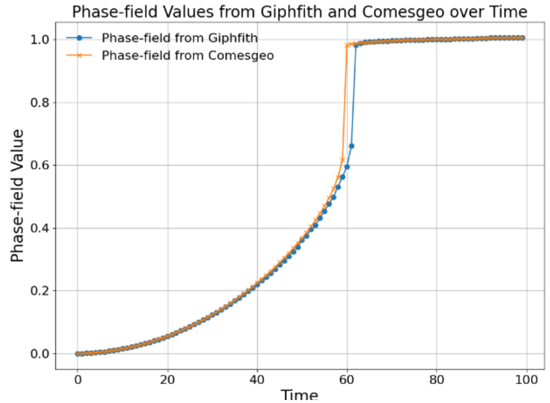
Traction of displacement



Phase-field result from Comes Geo

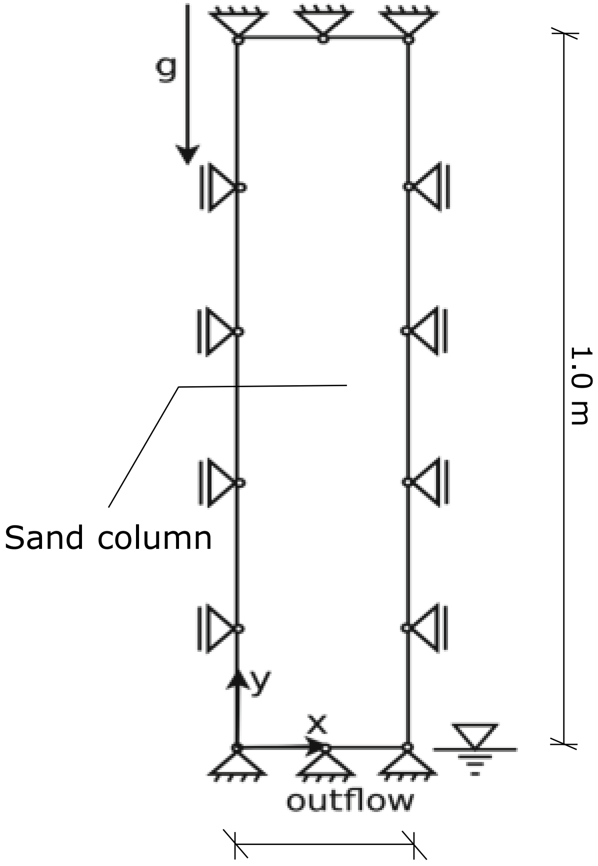
Phase-field result from Griphfith





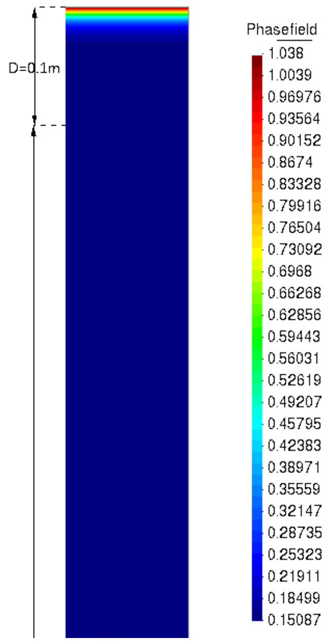
4. Current results of the work

Validation of the implementation: desaturation of a water saturated restrained column

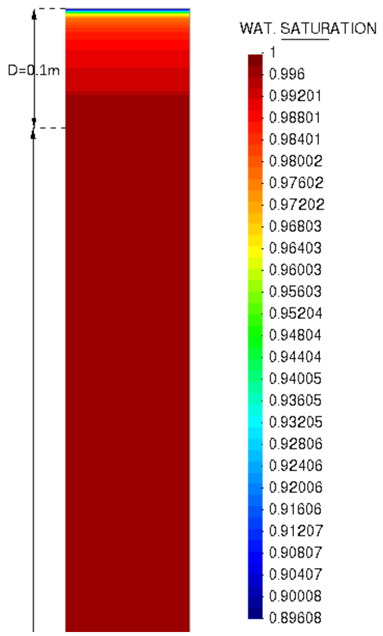


Geometry and boundary conditions

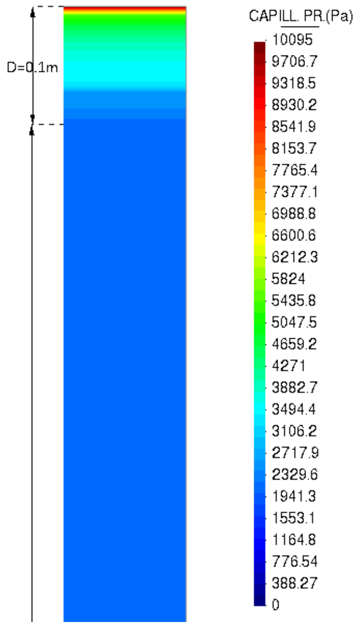
Hydro-mechanical problem *with crack phase-field*



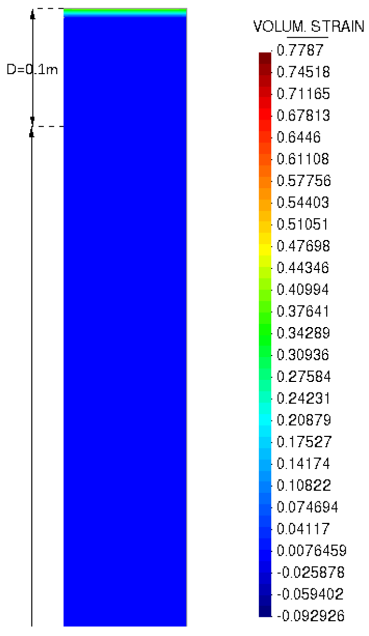
Phase-field



Water saturation



Capillary pressure



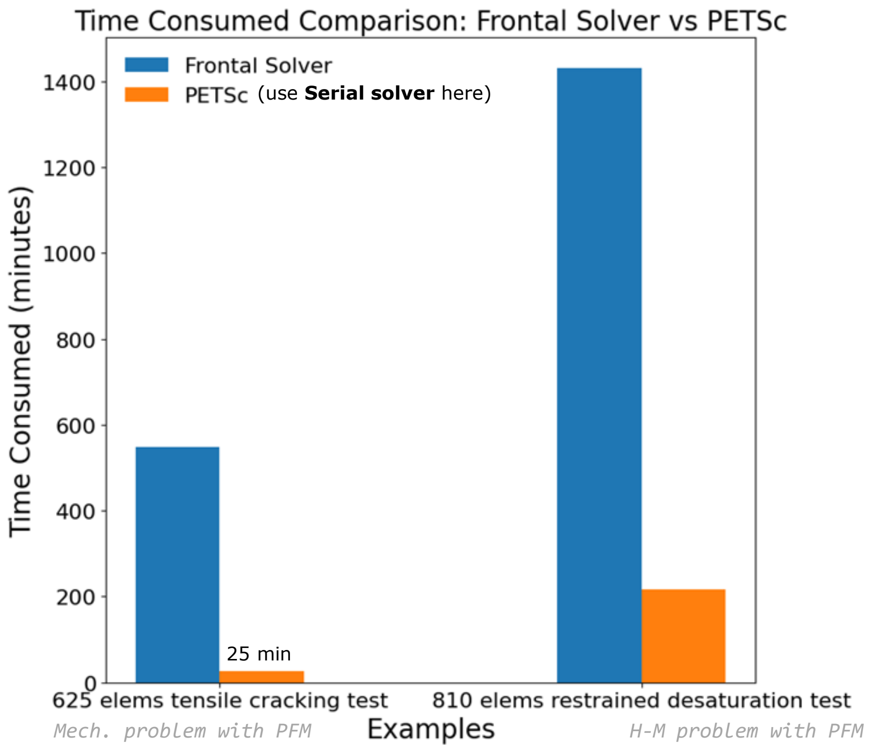
Volumetric strain

Contour plots at t ≈ 120 s.

4. Current results of the work

Acceleration of the computational time

A (parallel) direct sparse solver using `Cholesky factorization` was applied to solve the phase field equation instead of the original frontal solver by Bianco et al. 2003:



PETSc

An open-source FEM code package named:
the ***P**ortable, **E**xtensible **T**oolkit for **S**cientific **c**omputation*

Reference*:*

S. Balay, S. Abhyankar, M. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, A. Dener, V. Eijkhout, W. Gropp, et al., PETSc Users Manual, Argonne National Laboratory, 2019.

Bianco, M., et al. (2003). "A frontal solver tuned for fully coupled non-linear hygro-thermo-mechanical problems." International Journal for Numerical Methods in Engineering 57(13): 1801-1818.

5. Summary and future works

1. A numerical model able to study the nucleation and propagation of cracks induced by thermal effects in multiphase heterogenous porous materials has been implemented.

2. Validation performed solving: (i) a pure mechanical problem with crack phase-field (a tensile test in an inhomogeneous solid material) and (ii) a hydro-mechanical problem with crack phase-field (a restrained desaturation test).

3. A more efficient solver (PETSc package) has been introduced to solve the phase field evolution equation.

4. The THM crack Phase-field numerical model will be applied to study a thermal shock problem and a constrained desiccation problem.

5. The THM crack phase-field model will be extended to dynamics, and experimental tests will be studied both in quasi-statics and dynamic loading conditions.

6. The model will be also extended to ductile fracture.

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Publication and secondements

Conference submitted:

35th ALERT Workshop (30 Sep. to 02 Oct. 2024), Aussois (France). Poster session: Multiphysics modelling of desaturation cracks in non-isothermal multiphase porous media. (Book of abstracts: in print, with ISBN)

Secondment completed:

3 months at ETH Zurich hosted by Prof. Laura De Lorenzis has been done.

Conference planned:

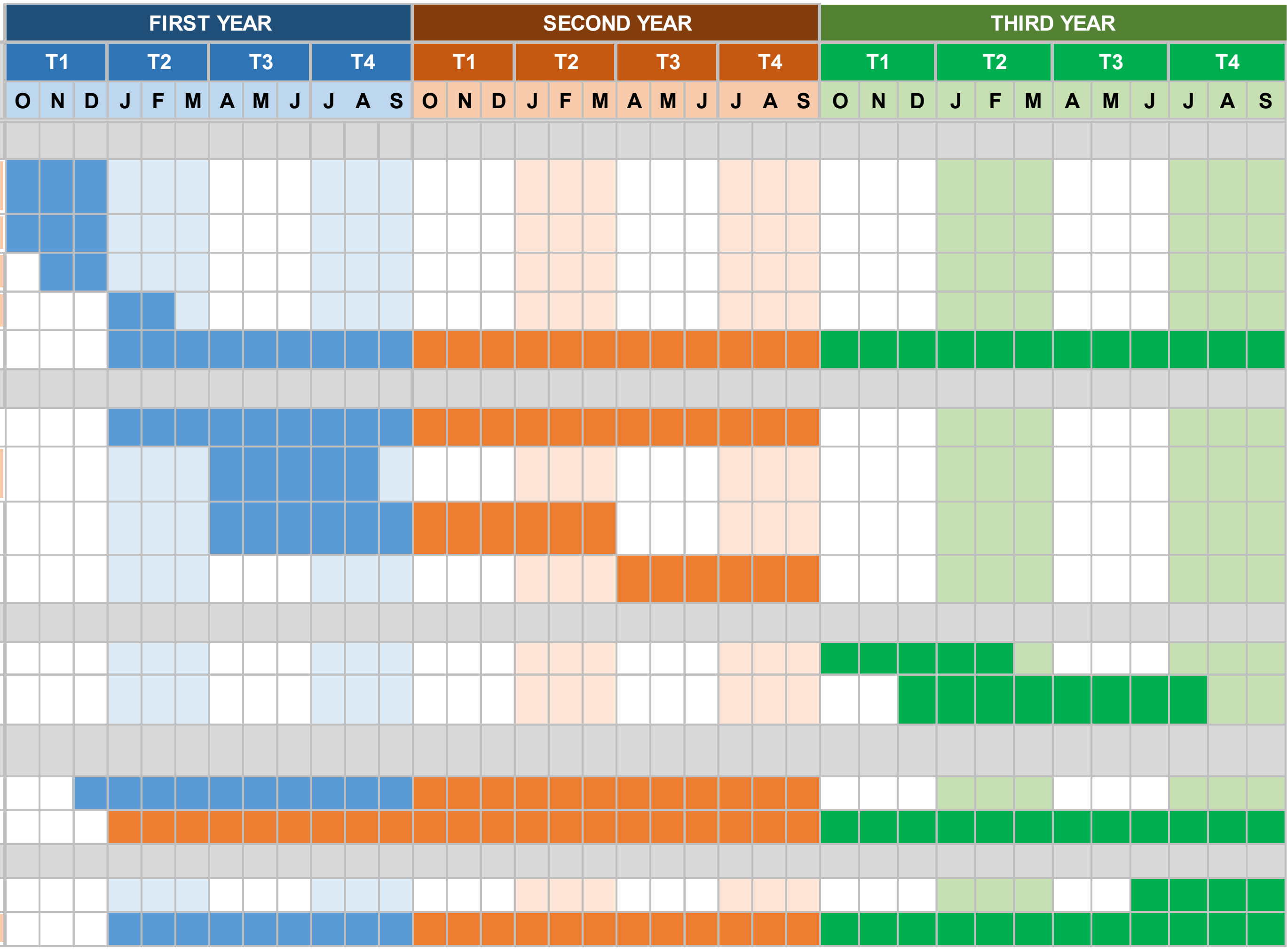
5th International Conference on Computational Methods for Multi-scale, Multi-uncertainty and Multi-physics Problems, Porto, Portugal, 2-4 July 2025

Secondment planned:

Another 3 months at ETH Zurich hosted by Prof. Laura De Lorenzis has been planned in 2025.

GANNT chart

WBS NUMBER	TASK TITLE	% OF TASK COMPL
1	**Study of the state of the art**	
1.1	State-of-art report on experimental desiccation and thermal cracks and on modelling cracks in multiphase porous media within the crack phase-field approach	100%
1.2	Mechanics of non-isothermal variably saturated porous media	100%
1.3	Fracture mechanics with the variational phase-field approach	100%
1.4	Computational geomechanics and fracture mechanics	100%
1.5	Update of the state-of-art report	33%
2	**Development a THM (Thermo-Hydro-Mechanical) crack phase-field numerical model**	
2.1	Implementation of the numerical finite element code	90%
2.2	Implementation of Quad8 element in *Griphfith* of ETH to be compatible with *ComesGeo* code in Padua	100%
2.3	Validation of the phase-field part of the code with analytical, numerical and experimental tests from literature	80%
2.4	Validation of the coupled phase-field THM model with analytical, numerical and experimental tests from literature	60%
3	**Extension of the THM crack phase-field model**	
3.1	Implementation of the dynamics at low frequencies and simulation of experimental tests	0%
3.2	Implementation of ductile fracture and simulation of experimental tests to study quasi-statics and dynamics fracture	0%
4	**Educational activities**	
4.1	Exams	90%
4.2	Conferences and seminars	90%
5	**Writing of the PhD thesis and reports of the research progress**	
5.1	Writing of the PhD thesis	0%
5.2	Writing of the report of the research progress	5%



Thanks for the attention

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