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ANNI



UNIVERSITÀ  
DEGLI STUDI  
DI PADOVA

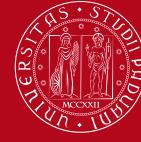
# Multiphysics modelling of thermal cracks in multiphase heterogenous porous materials

**PhD Candidate: Zechao Chen -- 38th**

Admission to the second year - 13/09/2023

**Supervisor: Prof. Lorenzo Sanavia   Co-supervisor: Prof. Laura De Lorenzis, ETH**

PhD Course in Sciences, Technologies And Measurements For Space

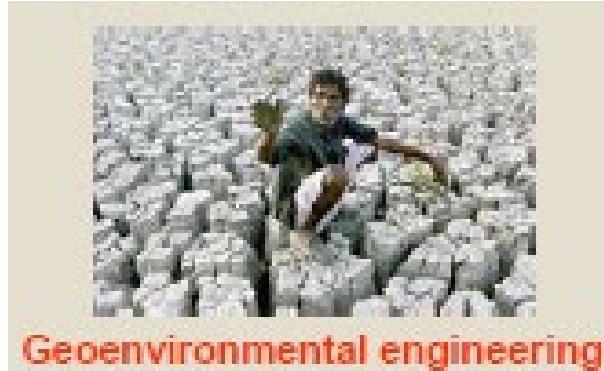


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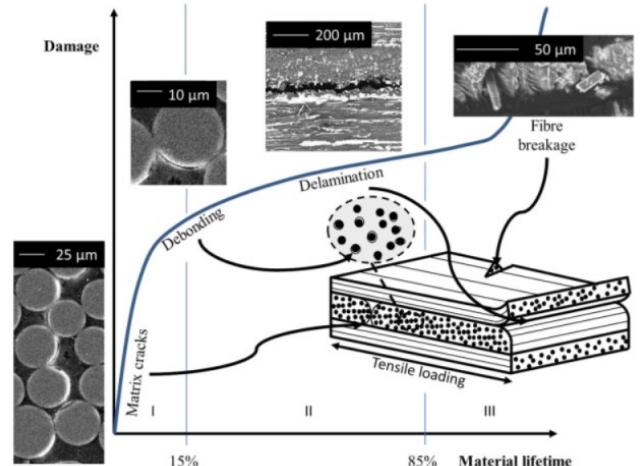
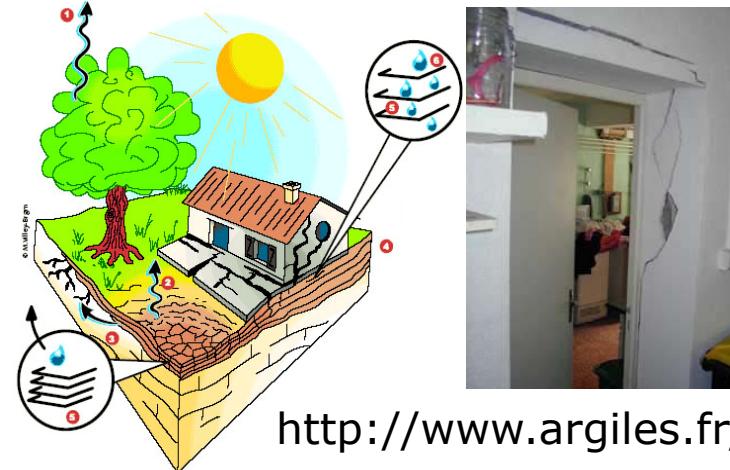
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# Introduction

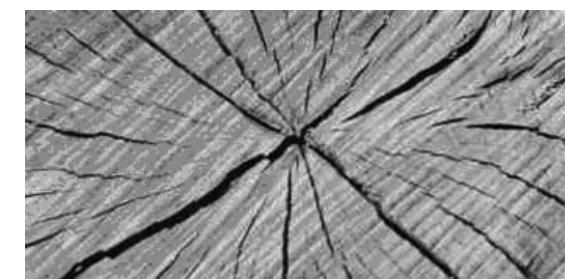
## Motivation: cracks due to hydro-thermal effects



*Desiccation (Laloui 2009)*

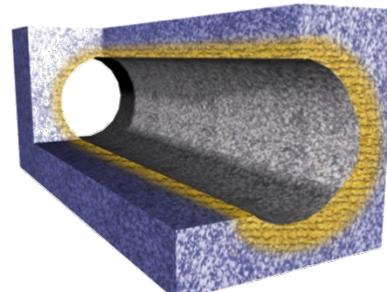


Damage in composite laminates  
[doi.org/10.1007/s10853-018-2045-6](https://doi.org/10.1007/s10853-018-2045-6)

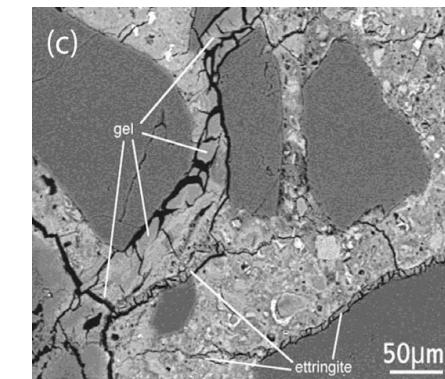


Cracks in wood

Desaturation/cracks development of EDZ (Excavation Damaged Zone)



Deep nuclear waste disposals

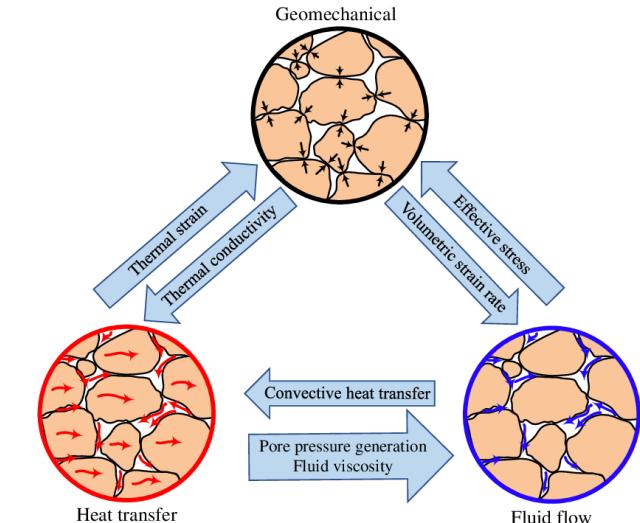
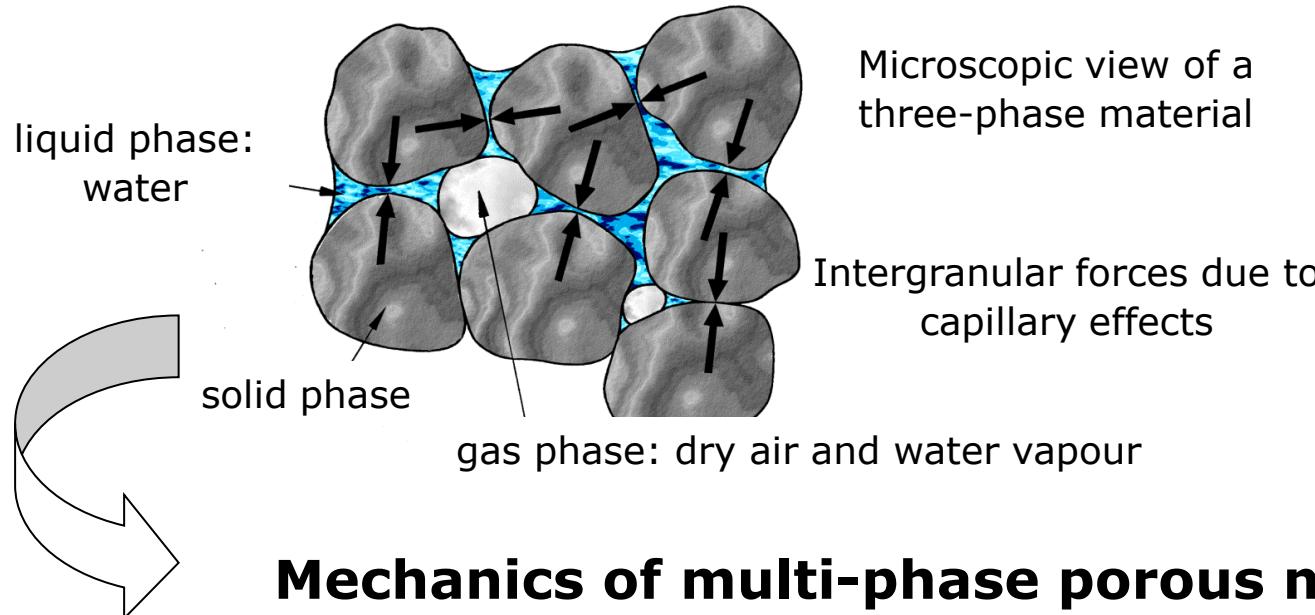


ASR (Alkali-Silica Reaction) shrinkage-induced cracking in concrete

# Research background

## Multi-phase porous material

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



## 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.

# Research background

## Multi-phase porous material

Equilibrium equations (mixture; quasi-statics):

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

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

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

- 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.

# Research background

## Multi-phase porous material

Dry air mass balance equation:

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

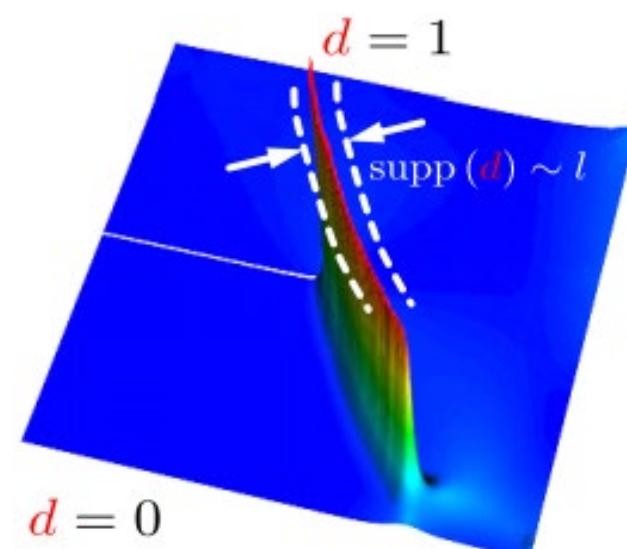
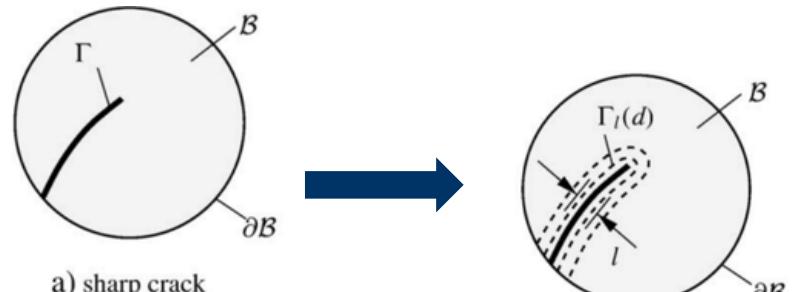
Energy balance equation (mixture):

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

- 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.

# Research background

## The Phase-Field Method (PFM) to fracture



### Key advantages

- Flexibility (initiation, propagation, merging, branching)
- Variational framework
- Simple implementation

### Disadvantages

- Fine mesh needed
- Efficiency/robustness of solution

- [SwissMech Seminars Archive – SwissMech Seminars](#)

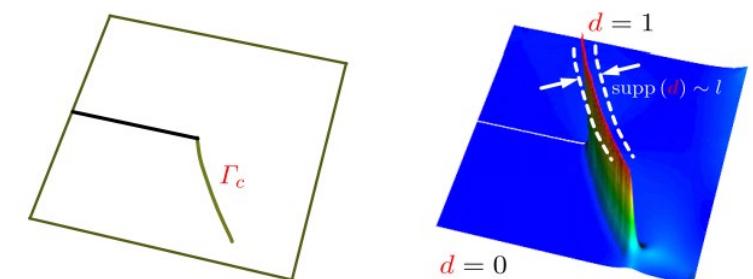
# Research background

## The Phase-Field Method (PFM) to fracture

### Sharp crack: (variational reformulation of) Griffith

$$\min_{\mathbf{u} \in \mathcal{U}_n(\Gamma_c), \Gamma_c \supseteq \Gamma_{cn-1}} \mathcal{E}(\mathbf{u}, \Gamma_c) = \underbrace{\int_{\Omega \setminus \Gamma_c} \psi(\varepsilon(\mathbf{u})) d\Omega}_{\text{elastic strain energy}} + \underbrace{G_c \mathbb{H}^{d-1}(\Gamma_c)}_{\text{fracture energy}} - \int_{\Omega} \mathbf{b}_n \cdot \mathbf{u} d\Omega - \int_{\partial \Omega_N} \mathbf{t}_n \cdot \mathbf{u} dS$$

Francfort and Marigo (1998)  
Mumford and Shah (1989)



### Diffusive crack: phase-field approach

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

Bourdin et al. (2000)  
Ambrosio and Tortorelli (2000)  
Braides (1998)

- [SwissMech Seminars Archive](#) – [SwissMech Seminars](#)

## The Phase-Field Method (PFM) to fracture

...with energy decomposition

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

*Amor et al. (2009)*

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

**Phase-field evolution equation**

$$-2l\Delta d + \frac{1}{2l}d = \frac{2(1-d)}{G_c} \mathcal{H} \quad \mathcal{H}(\mathbf{x}, t) := \max_{\tau \in [0, t]} \Psi^+(\varepsilon(\mathbf{x}, \tau))$$

$g(d)$  : degradation function

$\psi$ : elastic energy density function ( $\psi^+$  refers to tension and  $\psi^-$  is compression)

$G_c$  : fracture toughness

$w(d)$ : local damage function/dissipation function

$\ell$ : crack length scale parameter/ regularization length

$\nabla d$ : spatial gradient

$\mathbf{u}$ : displacement field

$c_w$ : normalization constant

$d$ : fracture phase field

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

# Project objectives

## Develop a THM (Thermo-Hydro-Mechanical) crack Phase-field numerical model

- Develop a numerical model able to study the nucleation and propagation of cracks induced by **thermal effects** in multiphase heterogenous porous materials.
- Merge 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** (the Grifhfit code for brittle fracture developed at ETH Zurich).
- After **validation with experiments** designed from the numerical modelling, the model will be further **extended**:
  - a) from quasi-statics to dynamics
- Application to study desiccation cracks in clayey materials and in heterogeneous composite materials.

# Work methodology

## Implementation strategy

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

- 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  $n = 0 : N-1$  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  $\mathbf{u}-p_w := \mathbf{U}_{n+1}(d_{n+1})$ ;
end
```

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



```

Initialization ( $t = t_0 = 0$ ):  $\bar{\mathbf{u}}, \bar{\mathbf{t}}, \bar{p}, \bar{q}, \bar{d}, \mathcal{H}, \mathbf{T} = 0$ ;
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  $\mathbf{u}-p_c-p_g-\mathbf{T} := \mathbf{U}_{n+1}(d_{n+1})$ ;
end
```

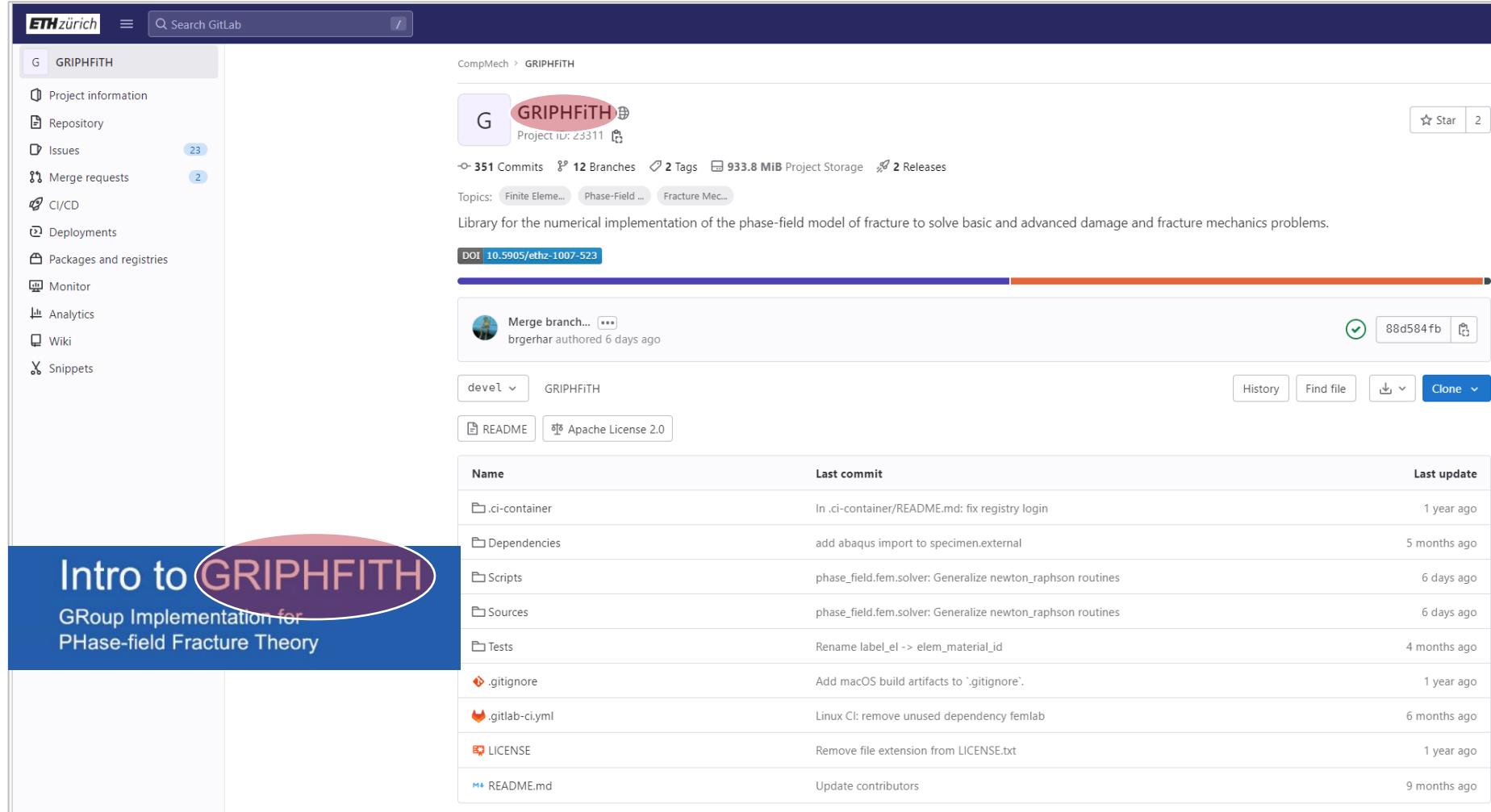
**Algorithm :** Algorithmic solution procedure for the  $\mathbf{u}$ - $p_c$ - $p_g$ - $\mathbf{T}$ - $d$  system

**Previous algorithm**

**New algorithm**

# Work methodology

## What has been done



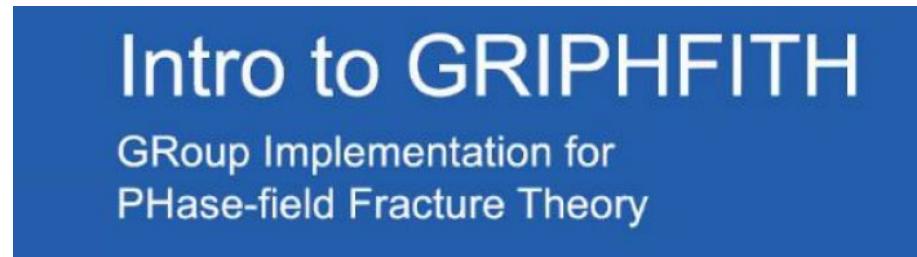
The screenshot shows the GitHub interface for the `GRIPHFiTH` repository. The sidebar on the left lists various project management sections: Project information, Repository, Issues (23), Merge requests (2), CI/CD, Deployments, Packages and registries, Monitor, Analytics, Wiki, and Snippets. The main content area displays the repository details for `CompMech / GRIPHFiTH`, including the project ID (23311), 351 Commits, 12 Branches, 2 Tags, 933.8 MIB Project Storage, and 2 Releases. Topics listed are Finite Element, Phase-Field, and Fracture Mechanics. A DOI link ([10.5905/ethz-1007-523](https://doi.org/10.5905/ethz-1007-523)) is provided. Below this, a commit history shows a merge branch from `brgher` 6 days ago. The repository structure includes `devel`, `GRIPHFiTH`, `README`, and `Apache License 2.0`. A detailed table of commits is shown, with the last commit being a fix for registry login. The repository was last updated 9 months ago.

| Name                        | Last commit  | Last update  |
|-----------------------------|--|--------------|
| <code>.ci-container</code>  | In <code>.ci-container/README.md</code> : fix registry login             | 1 year ago   |
| <code>Dependencies</code>   | add abaqus import to specimen.external                                   | 5 months ago |
| <code>Scripts</code>        | <code>phase_field.fem.solver</code> : Generalize newton_raphson routines | 6 days ago   |
| <code>Sources</code>        | <code>phase_field.fem.solver</code> : Generalize newton_raphson routines | 6 days ago   |
| <code>Tests</code>          | Rename label_el -> elem_material_id                                      | 4 months ago |
| <code>.gitignore</code>     | Add macOS build artifacts to <code>'.gitignore'</code> .                 | 1 year ago   |
| <code>.gitlab-ci.yml</code> | Linux CI: remove unused dependency femlab                                | 6 months ago |
| <code>LICENSE</code>        | Remove file extension from <code>LICENSE.txt</code>                      | 1 year ago   |
| <code>README.md</code>      | Update contributors  | 9 months ago |

# Work methodology

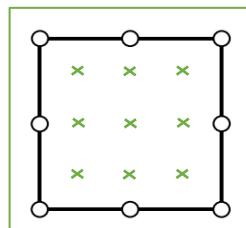
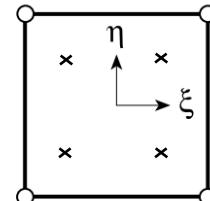
## What has been done

Implementation of Quad8 element in Grifhfit of ETH Zurich to be compatible with ComesGeo code in UNIPD

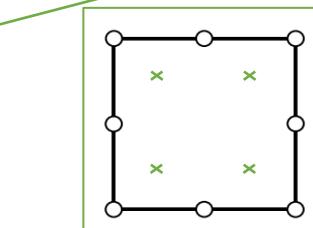


Fortran-Matlab  
Hybrid  
Programming  
source code

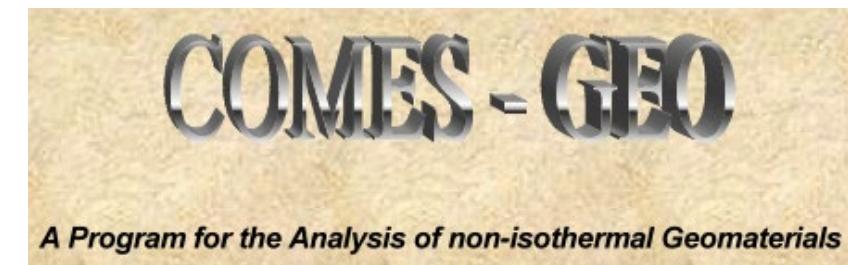
### GRIPHITH



Zechao Chen

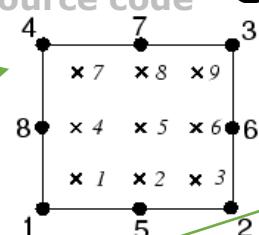


Multiphysics modelling of thermal cracks in multiphase heterogenous porous materials

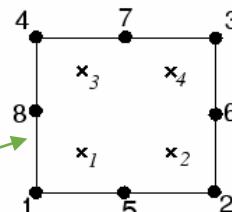


Fortran  
source code

### COMESGEO



Standard  
8-node element



Reduced-integration  
8-node element

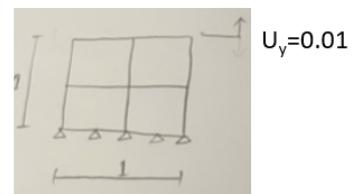
# Work methodology

## What has been done

- In new version of Grifhfit

```
# vtk DataFile Version 3.0
Solution
ASCII
DATASET UNSTRUCTURED_GRID
POINTS 21 float
Four elements--Quad4--4 Gauss points
 0.00000000000000E+000 0.00000000000000E+000 0.00000000000000E+000
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CELLS 4 20
 0 3
 1 4
 1 4
 2 5
 3 6
 4 7
 4 7
 5 8
CELL_TYPES 4
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 9
 9
 9
POINT_DATA 9
VECTORS Displacement float
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 -0.00000000000000 0.00500000000000 0.00000000000000
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 0.00000000000000 0.00000000000000 0.00000000000000
TENSORS Strain float
 -8.924500002264695E-019 4.336808699942014E-019 0.00000000000000E+000
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 5.312590645178968E-018 1.00000000000000E-002 0.00000000000000E+000
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 -1.849155480214625E-019 -1.517883041479705E-018 0.00000000000000E+000
 -1.517883041479705E-018 9.999999999999995E-003 0.00000000000000E+000
 0.00000000000000E+000 0.00000000000000E+000 0.00000000000000E+000
 17 # vtk DataFile Version 3.0
 18 Solution
 19 ASCII
 20 DATASET UNSTRUCTURED_GRID
 21 POINTS 21 float
 22 Four element--Quad8--4 Gauss points
 23 0.00000000000000E+000 0.00000000000000E+000 0.00000000000000E+000
 24 0.00000000000000E+000 0.25000000000000E+000 0.00000000000000E+000
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 44 1.00000000000000E+000 1.00000000000000E+000 0.00000000000000E+000
 45 POINT_DATA 21
 46 VECTORS Displacement float
 47 0.00000000000000 0.00000000000000 0.00000000000000
 48 -0.00000000000000 0.00500000000000 0.00000000000000
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 65 0.00000000000000 0.00000000000000 0.00000000000000
 66 0.00000000000000 0.00000000000000 0.00000000000000
 67 TENSORS Stress float
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 69 2.60208521396521E-018 1.00000000000000E-002 0.00000000000000E+000
 70 0.00000000000000E+000 0.00000000000000E+000 0.00000000000000E+000
 71 -9.215935959040582E-019 -5.75719552365952E-019 0.00000000000000E+000
 72 -6.76791482240479E-019 1.00000000000000E-002 0.00000000000000E+000
 73
```

Tensile problem



# Work methodology

## What has been done

Summary

Tensile Problem

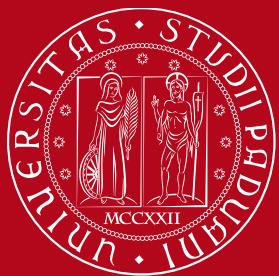
| Number Of Elements | Element Type | Gauss Points | New Version's Elasticity Problem | New Version's Brittle Fracture Problem | Problems |
|--------------------|--------------|--------------|----------------------------------|--|----------|
| 1                  | Quad 4       | 4            | ✓                                | ✓                                      |          |
| 1                  | Quad 8       | 4            | ✓                                | ✓                                      |          |
| 4                  | Quad 4       | 4            | ✓                                | ✓                                      | /        |
| 4                  | Quad 8       | 4            | ✓                                | ✓                                      |          |

Shear Problem

| Number Of Elements | Element Type | Gauss Points | New Version's Elasticity Problem | New Version's Brittle Fracture Problem | Problems   |
|--------------------|--------------|--------------|----------------------------------|--|--|
| 1                  | Quad 4       | 4            | ✓                                | ✓                                      |  |
| 1                  | Quad 8       | 4            | ✓                                | ✓                                      |  |
| 4                  | Quad 4       | 4            | ✓                                | ✓                                      |  |
| 4                  | Quad 8       | 4            | ✓                                | ✓                                      | can not compared with analytical solutions and the result of Quad4 |

# Thanks for the attention

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