Multiphysics modelling of thermal cracks in multiphase heterogenous porous materials

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Admission to the second year - 13/09/2023

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PhD Course in Sciences, Technologies And Measurements For Space

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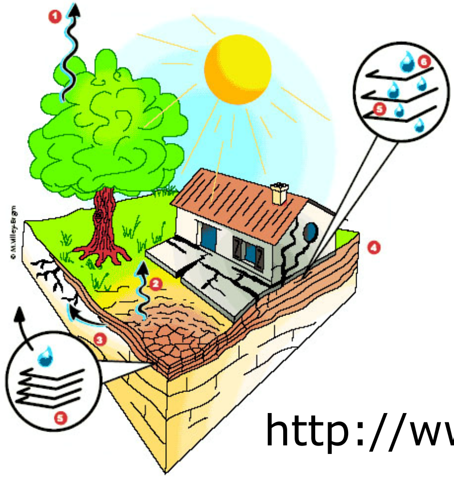
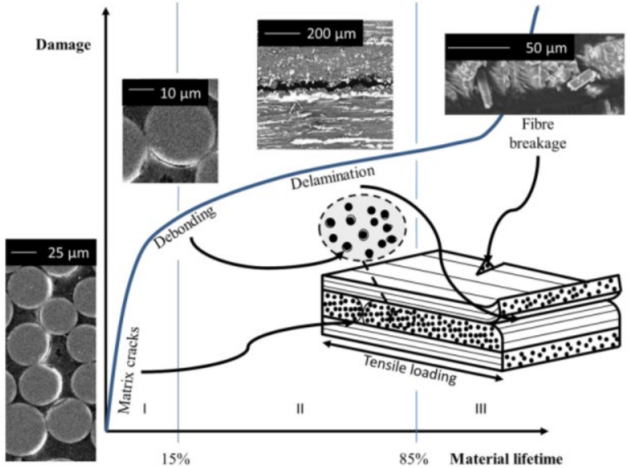
Introduction

Motivation: cracks due to hydro-thermal effects

Desiccation (Laloui 2009)



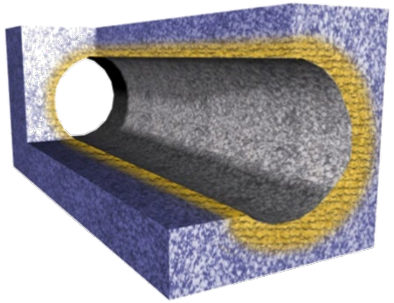
http://www.argiles.fr/

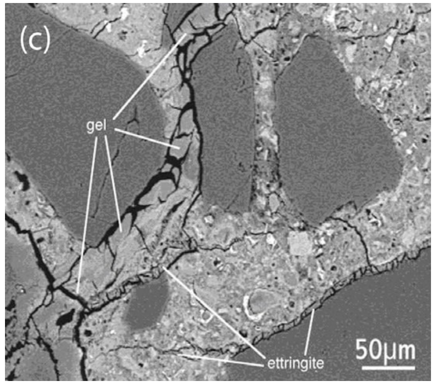


Damage in composite laminates doi.org/10.1007/s10853-018-2045-6

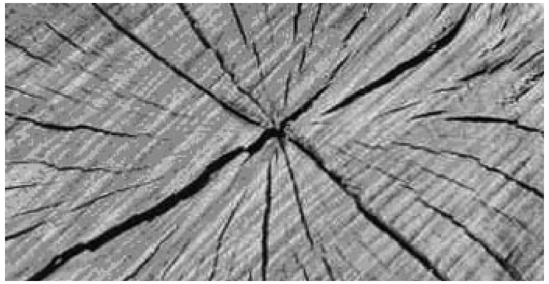
Desaturation/cracks developement of EDZ (Excavation Damaged Zone)

Deep nuclear waste disposals





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



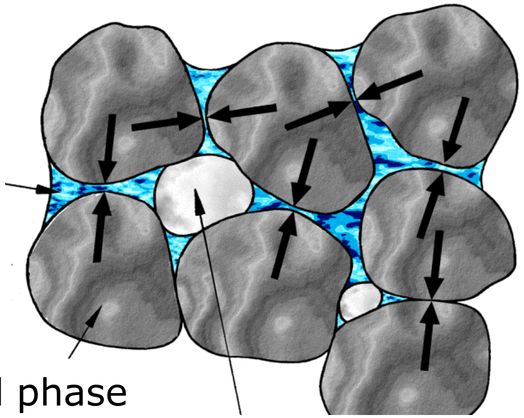
Cracks in wood

Research background

Multi-phase porous material

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

liquid phase: water

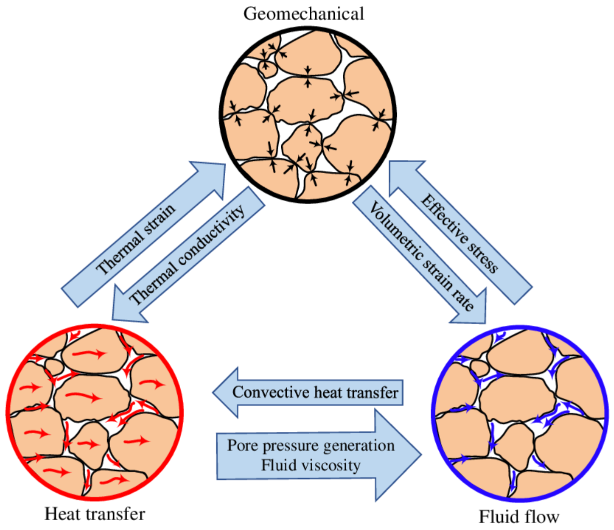


Microscopic view of a three-phase material

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.*

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):

$$n\left[\rho^{w} - \rho^{gw}\right]\left[\frac{\partial S_{w}}{\partial t}\right] + \left[\rho^{w}S_{w} - \rho^{gw}\left[1 - S_{w}\right]\right]div\left(\frac{\partial \mathbf{u}}{\partial t}\right) + \left[1 - S_{w}\right]n\left[\frac{\partial \rho^{gw}}{\partial t}\right]$$

$$-div\left(\rho^{g}\frac{M_{a}M_{w}}{M_{g}^{2}}\mathbf{D}_{g}^{gw}grad\left(\frac{\partial p^{gw}}{\partial p^{g}}\right)\right) + div\left(\rho^{w}\frac{\mathbf{k}k^{rw}}{\mu^{w}}\left[-grad(p^{g}) + grad(p^{c}) + \rho^{w}\mathbf{g}\right]\right)$$

$$+div\left(\rho^{gw}\frac{\mathbf{k}k^{rg}}{\mu^{g}}\left[-grad(p^{g}) + \rho^{g}\mathbf{g}\right]\right) - \beta_{swg}\frac{\partial T}{\partial t} = 0$$

- *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:

$$-n\rho^{ga}\left[\frac{\partial S_w}{\partial t}\right]+\rho^{ga}\left[1-S_w\right]div\left(\frac{\partial \mathbf{u}}{\partial t}\right)+nS_g\frac{\partial \rho^{ga}}{\partial t}-div\left(\rho^g\frac{M_aM_w}{M_g^2}\mathbf{D}_g^{ga}\,grad\left(\frac{p^{ga}}{p^g}\right)\right)$$

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

Energy balance equation (mixture):

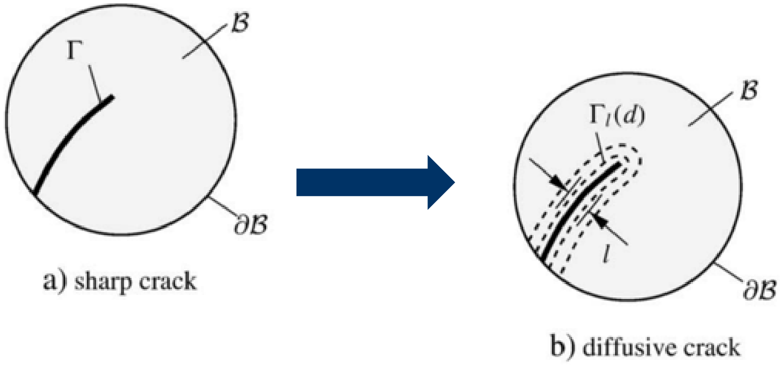
$$\left(\rho C_p\right)_{eff}\frac{\partial T}{\partial t}+\rho^wC_p^w\left(\frac{\mathbf{k}k^{rw}}{\mu^w}\left[-grad(p^g)+grad(p^c)+\rho^w\mathbf{g}\right]\right)\cdot grad(T)$$

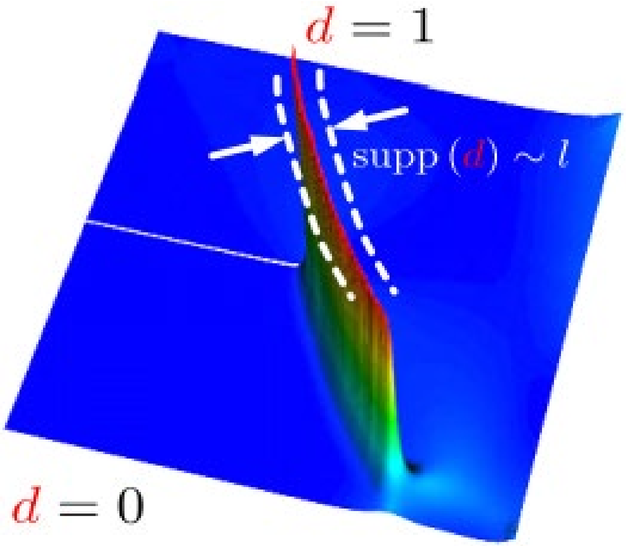
$$+\rho^gC_p^g\left(\frac{\mathbf{k}k^{rg}}{\mu^g}\left[-grad(p^g)+\rho^g\mathbf{g}\right]\right)\cdot grad(T)-div\left(\chi_{eff}\,grad(T)\right)=-\dot{m}_{vap}\,\Delta H_{vap}$$

- *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.*

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

The Phase-Field Method (PFM) to fracture

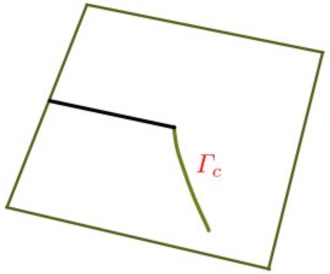
Sharp crack: (variational reformulation of) Griffith

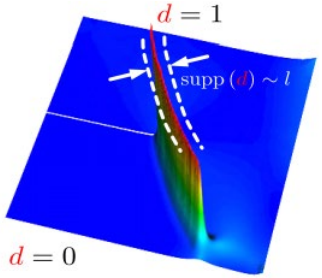
$$\min_{\mathbf{u}\in\mathcal{U}_n(\Gamma_c),\Gamma_c\supseteq\Gamma_{cn-1}} \mathcal{E}(\mathbf{u},\Gamma_c) = \underbrace{\int_{\Omega\setminus\Gamma_c} \psi(\varepsilon(\mathbf{u}))d\Omega}_{\text{elastic strain energy}} + \underbrace{G_c\mathbb{H}^{d-1}(\Gamma_c)}_{\text{fracture energy}} - \int_\Omega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

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

regularization

$\ell\to 0$
Γ−convergence





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*

Research background

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

$g(d)$: degradation function

G_c : fracture toughness

ℓ: crack length scale parameter/ regularization length

$\mathbf{u}$: displacement field

d: fracture phase field

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

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

∇d: spatial gradient

c_w: normalization constant

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

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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 Griphfith 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 $n = 0 : N\text{-}1$ **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

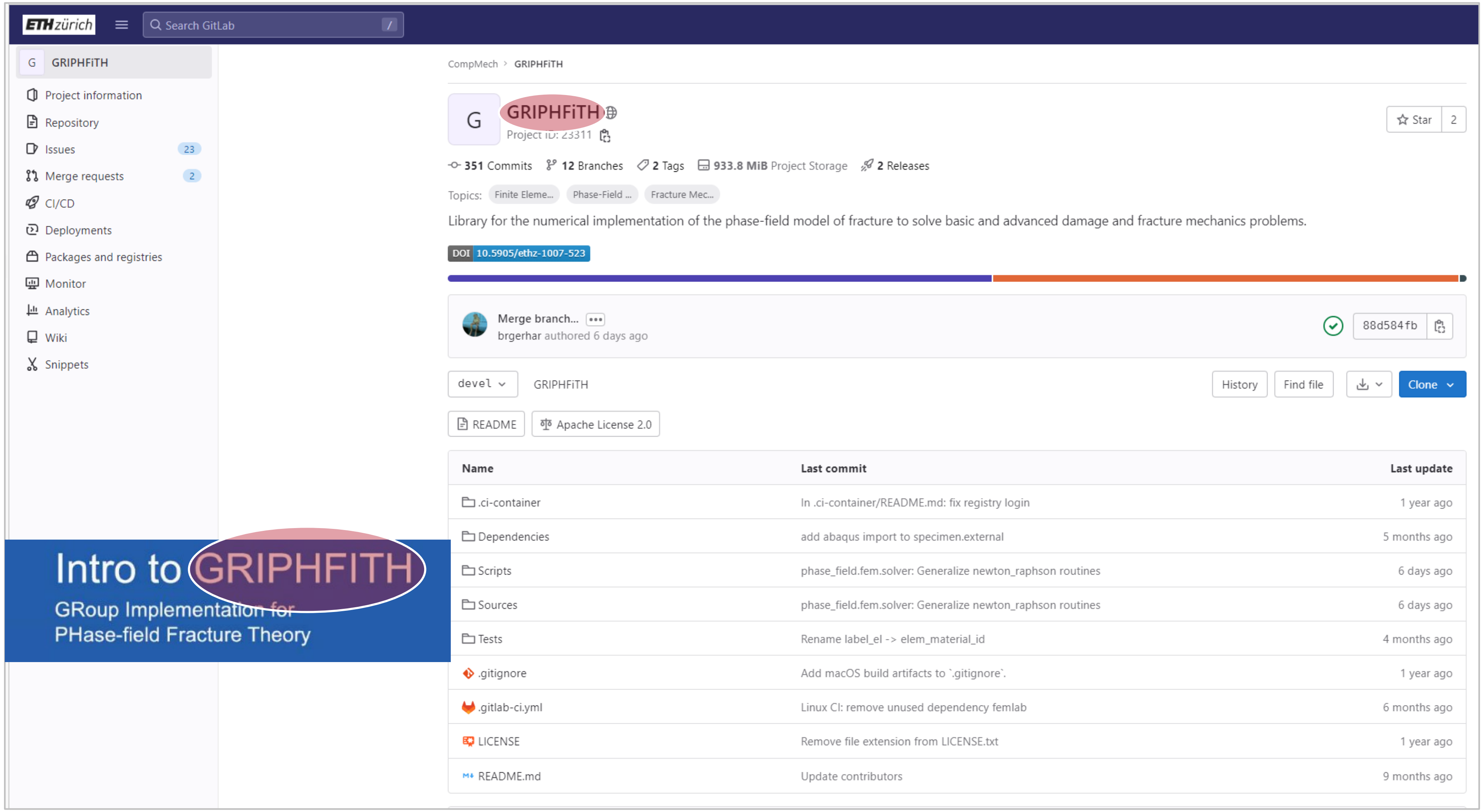
Previous algorithm

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 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

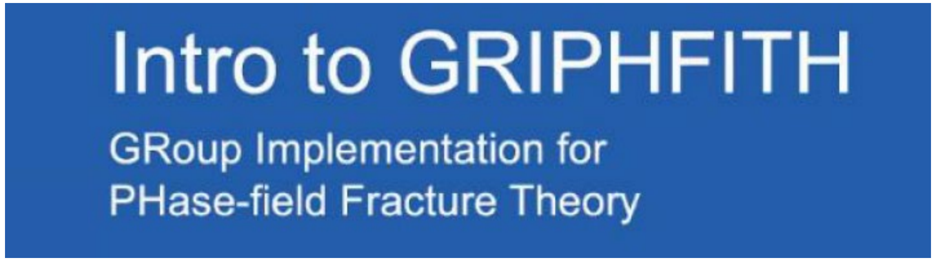
What has been done

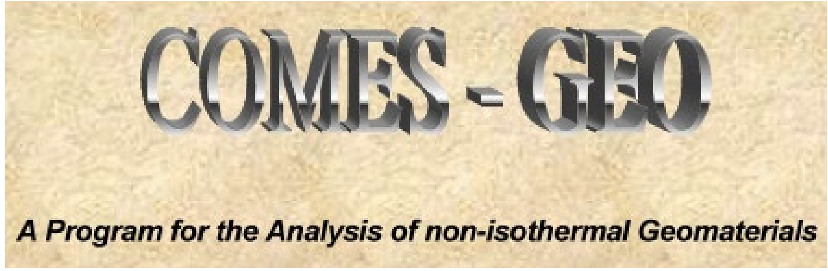


Work methodology

What has been done

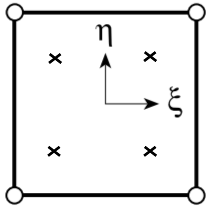
Implementation of Quad8 element in Griphfith of ETH Zurich to be compatible with ComesGeo code in UNIPD





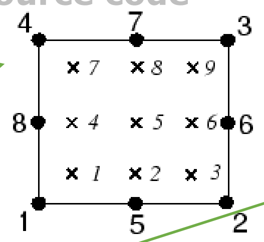
Fortran-Matlab Hybrid Programming source code

GRIPHFITH

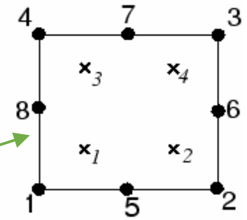


Fortran source code

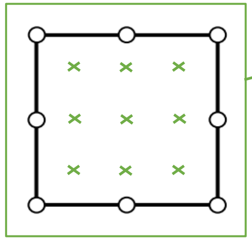
COMESGEO

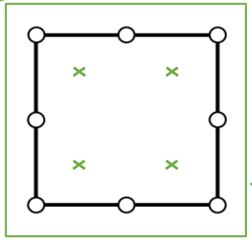


Standard 8-node element



Reduced-integration 8-node element





Work methodology

What has been done

- In new version of Griphfith

Four elements--Quad4--4 Gauss points

```
# vtk DataFile Version 3.0
Solution
ASCII
DATASET UNSTRUCTURED_GRID
POINTS        9 float
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
  0.000000000000000E+000  0.500000000000000       0.000000000000000E+000
  0.000000000000000E+000   1.00000000000000       0.000000000000000E+000
  0.500000000000000       0.000000000000000E+000  0.000000000000000E+000
  0.500000000000000       0.500000000000000       0.000000000000000E+000
  0.500000000000000        1.00000000000000       0.000000000000000E+000
   1.00000000000000       0.000000000000000E+000  0.000000000000000E+000
   1.00000000000000       0.500000000000000       0.000000000000000E+000
   1.00000000000000        1.00000000000000       0.000000000000000E+000
CELLS         4        20
                       4                      0                      3
                       4                      1
                       4                      1                      4
                       5                      2
                       4                      3                      6
                       7                      4
                       4                      4                      7
                       8                      5
CELL_TYPES          4
                       9
                       9
                       9
                       9
POINT_DATA          9
VECTORS Displacement float
             0.000000000000000              0.000000000000000              0.000000000000000
            -0.000000000000000              0.005000000000000              0.000000000000000
             0.000000000000000              0.010000000000000              0.000000000000000
            -0.000000000000000              0.000000000000000              0.000000000000000
            -0.000000000000000              0.005000000000000              0.000000000000000
             0.000000000000000              0.010000000000000              0.000000000000000
            -0.000000000000000              0.000000000000000              0.000000000000000
            -0.000000000000000              0.005000000000000              0.000000000000000
             0.000000000000000              0.010000000000000              0.000000000000000
TENSORS Strain float
 -8.924500002264695E-019  4.336808689942014E-019  0.000000000000000E+000
  4.336808689942014E-019  1.000000000000000E-002  0.000000000000000E+000
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000

  1.005061465297237E-019 -2.168404344971009E-018  0.000000000000000E+000
 -2.168404344971009E-018  1.000000000000001E-002  0.000000000000000E+000
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000

 -1.162328814093078E-034 -4.770489558936217E-018  0.000000000000000E+000
 -4.770489558936217E-018  9.999999999999998E-003  0.000000000000000E+000
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000

 -5.386827741239659E-019  7.589415207398522E-019  0.000000000000000E+000
  7.589415207398522E-019  1.000000000000000E-002  0.000000000000000E+000
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000

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  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000

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  5.312590645178968E-018  1.000000000000000E-002  0.000000000000000E+000
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000

 -1.849155480214625E-019 -1.517883041479705E-018  0.000000000000000E+000
 -1.517883041479705E-018  9.999999999999995E-003  0.000000000000000E+000
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
```

Four element--Quad8--4 Gauss points

```
# vtk DataFile Version 3.0
Solution
ASCII
DATASET UNSTRUCTURED_GRID
POINTS       21 float
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
  0.000000000000000E+000  0.250000000000000       0.000000000000000E+000
  0.000000000000000E+000  0.500000000000000       0.000000000000000E+000
  0.000000000000000E+000  0.750000000000000       0.000000000000000E+000
  0.000000000000000E+000   1.00000000000000       0.000000000000000E+000
  0.250000000000000       0.000000000000000E+000  0.000000000000000E+000
  0.250000000000000       0.500000000000000       0.000000000000000E+000
  0.250000000000000        1.00000000000000       0.000000000000000E+000
  0.500000000000000       0.000000000000000E+000  0.000000000000000E+000
  0.500000000000000       0.250000000000000       0.000000000000000E+000
  0.500000000000000       0.500000000000000       0.000000000000000E+000
  0.500000000000000       0.750000000000000       0.000000000000000E+000
  0.500000000000000        1.00000000000000       0.000000000000000E+000
  0.750000000000000       0.000000000000000E+000  0.000000000000000E+000
  0.750000000000000       0.500000000000000       0.000000000000000E+000
  0.750000000000000        1.00000000000000       0.000000000000000E+000
   1.00000000000000       0.000000000000000E+000  0.000000000000000E+000
   1.00000000000000       0.250000000000000       0.000000000000000E+000
   1.00000000000000       0.500000000000000       0.000000000000000E+000
   1.00000000000000       0.750000000000000       0.000000000000000E+000
   1.00000000000000        1.00000000000000       0.000000000000000E+000
CELLS        4       36
                   8                  0                  2                 10                  8
                   8                  2                  4                 12                 10
                   8                  8                 10                 18                 16
                   8                 10                 12                 20                 18
CELL_TYPES        4
                    9
                    9
                    9
                    9
CELL_DATA        4
SCALARS MAT_ID int 1
LOOKUP_TABLE default
  1
  1
  1
  1
POINT_DATA       21
VECTORS Displacement float
           0.000000000000000            0.000000000000000            0.000000000000000
          -0.000000000000000            0.002500000000000            0.000000000000000
          -0.000000000000000            0.005000000000000            0.000000000000000
           0.000000000000000            0.007500000000000            0.000000000000000
           0.000000000000000            0.010000000000000            0.000000000000000
          -0.000000000000000            0.000000000000000            0.000000000000000
           0.000000000000000            0.005000000000000            0.000000000000000
           0.000000000000000            0.010000000000000            0.000000000000000
          -0.000000000000000            0.000000000000000            0.000000000000000
          -0.000000000000000            0.002500000000000            0.000000000000000
           0.000000000000000            0.005000000000000            0.000000000000000
           0.000000000000000            0.007500000000000            0.000000000000000
           0.000000000000000            0.010000000000000            0.000000000000000
          -0.000000000000000            0.000000000000000            0.000000000000000
          -0.000000000000000            0.005000000000000            0.000000000000000
           0.000000000000000            0.010000000000000            0.000000000000000
          -0.000000000000000            0.000000000000000            0.000000000000000
          -0.000000000000000            0.002500000000000            0.000000000000000
          -0.000000000000000            0.005000000000000            0.000000000000000
           0.000000000000000            0.007500000000000            0.000000000000000
           0.000000000000000            0.010000000000000            0.000000000000000
TENSORS Stress float
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  2.602085213965214E-018  1.000000000000000E-002  0.000000000000000E+000
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000

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```
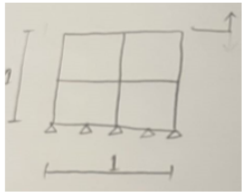

Tensile problem



U_y=0.01

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	✓	✓	can not compared with analytical solutions and the result of Quad4
1	Quad 8	4	✓	✓	
4	Quad 4	4	✓	✓	
4	Quad 8	4	✓	✓	

Thanks for the attention

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