Numerical modelling of multiphysics couplings and the strain localization

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Failure in soils and rocks is almost always associated with fractures and/or shear bands developing in the geomaterial.

Shear banding occurs frequently (at many scales) and is the source of many soil and rock engineering problems:

natural or human-made slopes or excavations, unstable rock masses, embankments or dams, tunnels and mine galleries, boreholes driven for oil production, repositories for nuclear waste disposal
In situ observations of shear banding and/or faulting are made frequently at many scales.

Large scale: railway tracks after an earthquake in Turkey
Human-made slope along E42 exit road

*Bierset (Belgium) 1998 – Courtesy C. Schroeder*
Nuclear waste disposal

*Fractures observed during the construction of the connecting gallery at the URL in Mol. Vertical cross section through the gallery showing the fracturation pattern around it, as deduced from the observations (from Alheid et al. 2005)*
Localized rupture in sandstone samples under different confining pressures (Bésuelle et al., 2000)

Experimental characterisation of the localisation phenomenon inside a Vosges sandstone in a triaxial cell

Experimental observations: biaxial test

Experimental set-up & a typical test
INTRODUCTION

Failure in soils and rocks is almost always associated with fractures and/or shear bands developing in the geomaterial.

Shear banding occurs frequently (at many scales) and is the source of many soil and rock engineering problems:

natural or human-made slopes or excavations, unstable rock masses, embankments or dams, tunnels and mine galleries, boreholes driven for oil production, repositories for nuclear waste disposal

In geomaterials, the understanding of failure processes is more complex by the fact that soils and rocks are multiphase porous materials where different multiphysical processes take place.

The application problem will be the nuclear waste disposal in deep geological layers.
Outline:

- Introduction
- Theoretical tools
- Numerical models
- Numerical application
- Conclusions
Experimental evidence:

- Initial state
- Homogeneous strain field
- Localized strain field
Theoretical background

Following the previous works by (Hadamard, 1903), (Hill, 1958) and (Mandel, 1966), Rice and co-workers (Rice, 1976, Rudnicki et al., 1975) have proposed the so-called Rice criterion.
Theoretical concepts

Static condition: \( n \left( \dot{\sigma}^1 - \dot{\sigma}^0 \right) = 0 \)

Kinematic condition: \( L^1 = L^0 + \Delta L \)

Constitutive law: \( \dot{\sigma} = C : L \)

When it is assumed that \( C^1 = C^0 = C \), no trivial solution if and only if:

\[
\det(nCn) \leq 0
\]
Theoretical concepts

Constitutive law in principal axis:

\[
\begin{align*}
\begin{bmatrix}
\dot{\sigma}_{11} \\
\dot{\sigma}_{22} \\
\dot{\sigma}_{12}
\end{bmatrix} &= \begin{bmatrix}
C_{11} & C_{12} & 0 \\
C_{21} & C_{22} & 0 \\
0 & 0 & 2G_{12}
\end{bmatrix}
\begin{bmatrix}
L_{11} \\
L_{22} \\
L_{12}
\end{bmatrix}
\end{align*}
\]

Static condition:

\[
\left(\dot{\sigma}_{ij}^1 - \dot{\sigma}_{ij}^0\right) n_j = 0
\]

\[
\begin{align*}
\left(\dot{\sigma}_{11}^1 - \dot{\sigma}_{11}^0\right) n_1 + \left(\dot{\sigma}_{12}^1 - \dot{\sigma}_{12}^0\right) n_2 &= 0 \\
\left(\dot{\sigma}_{21}^1 - \dot{\sigma}_{21}^0\right) n_1 + \left(\dot{\sigma}_{22}^1 - \dot{\sigma}_{22}^0\right) n_2 &= 0
\end{align*}
\]

Kinematic condition:

\[
L_{ij}^1 = L_{ij}^0 + g_i n_j
\]

Combining the three previous relationship yields:

If \( C^1 = C^0 = C \):

\[
\begin{align*}
\left(C_{11} g_1 n_1 + C_{12} g_2 n_2 \right) n_1 + G_{12} \left(g_1 n_2 + g_2 n_1 \right) n_2 &= 0 \\
G_{12} \left(g_1 n_2 + g_2 n_1 \right) n_1 + \left(C_{21} g_1 n_1 + C_{22} g_2 n_2 \right) n_2 &= 0
\end{align*}
\]
Theoretical concepts

\[
\begin{align*}
\left( C_{11} n_1^2 + G_{12} n_2^2 \right) g_1 + \left( C_{12} n_1 n_2 + G_{12} n_2 n_1 \right) g_2 &= 0 \\
\left( C_{21} n_1 n_2 + G_{12} n_2 n_1 \right) g_1 + \left( C_{22} n_2^2 + G_{12} n_1^2 \right) g_2 &= 0
\end{align*}
\]

When it is assumed that \( C^1 = C^0 = C \), no trivial solution if and only if: \( \det(nCn) \leq 0 \)

\[
\left( C_{11} G_{12} \right) n_1^4 + \left( C_{22} G_{12} \right) n_2^4 + \left( C_{11} C_{22} - 2 C_{12} G_{12} - C_{12}^2 \right) n_1^2 n_2^2 = 0
\]

\[
n_1^4 \left( a_1 z^4 + a_3 z^2 + a_5 \right) = 0 \quad z = \frac{n_2}{n_1}
\]

For a constitutive law written in cartesian axis:

\[
n_1^4 \left( a_1 z^4 + a_2 z^3 + a_3 z^2 + a_4 z + a_5 \right) = 0
\]
Extension to multiphysical context, mainly in hydro mechanical coupling:

Loret and co-workers (Loret et al., 1991) showed that for hydromechanical problems the condition of localization depends only on the **drained properties** of the medium.

In coupled problems much more complex localization pattern can be obtained, at least theoretically (Vardoulakis, 1996).
Which information can provide these theoretical tools?

For element test, the tools allow you to check if and when the constitutive model is able to predict the localization direction observed at the laboratory.

For boundary value problems, they provide you the stress state when bifurcation may arise and the direction of potential bifurcation (fracturation). Be aware that the Rice criterion is a local one!
Example n°1

Skeleton mechanical behaviour

Linear elasticity: \( E_0 \) et \( \nu_0 \)

Drucker Prager criterion:

\[
F \equiv \sqrt{\frac{3}{2}} II \hat{\sigma} + m \left( I_\sigma - \frac{3c}{\tan \phi} \right) = 0
\]

\[
m = \frac{2 \sin \phi}{3 - \sin \phi}
\]

\[
c = c_0 f(\gamma^p)
\]

Associated softening plasticity (decrease of cohesion):

\[
f(\gamma^p) = \left(1 - (1 - \alpha) \frac{\gamma^p}{\gamma_R^p}\right)^2 \text{ si } 0 < \gamma^p < \gamma_R^p
\]

\[
= \alpha^2 \text{ si } \gamma^p \geq \gamma_R^p
\]
Softening behaviour: localization effects are very important.
Theoretical concepts

First stress invariant [MPa]

Second deviatoric stress invariant [MPa]

-8 -6 -4 -2 0 2 4 6 8 10

First stress invariant [MPa]

0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5

Elément 1
Elément 195
Elément 196
Surface initiale
Surface finale
NL Courbe F-d
Max Courbe F-d
Bifurcation
Theoretical concepts

Softening behaviour: localization effects are very important.

Bifurcation analysis thanks to the Rice criterion (Acoustic tensor)

\[
\det\left(\Lambda(\vec{n})\right) = n_1^4 \left(a_1 z^4 + a_2 z^3 + a_3 z^2 + a_4 z + a_5\right) \leq 0
\]

Acoustic tensor determinant

Diagram showing curves labeled Elastique, 1er pas plastique, Pas avant Bif, Pas après bif, and Pas 150.
Theoretical concepts

Plastic point

Bifurcation dir.

Bifurcation cones
Theoretical concepts

Plastic point

Bifurcation dir.

Bifurcation cones
The Rice criterion provides us the information on when and how localization may appear. Do we have any problem to model such phenomenon with classical finite element method?

Let’s consider the modelling of a biaxial test with a defect triggering the localization, first without any hydromechanical effect.
Theoretical concepts

Introduction

Theory

Models

Application

Conclusions
The post peak behaviour depends on the mesh size!
Example n°2

Let’s consider now a coupled modelling:

- Cylindrical cavity without retaining structure
- Anisotropic initial state of stress
- Geometrical dimensions: *Internal radius 3 m*
  *Mesh length 60 m*

**Choice:**

- *Symmetry of the problem is assumed*
- *894 elements – 2647 nodes – 7941 dof*
Example of EDZ around a cavity

\[ \sigma_{xx} = \sigma_{zz} = -7.74 \text{MPa} \]
\[ \sigma_{yy} = -11.64 \text{MPa} \]
\[ p_w = 4.7 \text{MPa} \]

\[
\begin{cases}
0 \leq t \leq T \\
\sigma_{xx} = \sigma_{xx}' - b S_{rw} p_w = -11.5 \left( 1 - \frac{t}{T} \right) \text{MPa} \\
\sigma_{yy} = \sigma_{yy}' - b S_{rw} p_w = -15.4 \left( 1 - \frac{t}{T} \right) \text{MPa} \\
p_w = 4.7 \left( 1 - \frac{t}{T} \right) \text{MPa} \\
t > T \\
\sigma_{xx} = \sigma_{yy} = p_w = 0
\end{cases}
\]

\[ T = 1.5 \text{ Ms (17 days)} \]
\[ t_{\text{total}} = 300 \text{ Ms (9.5 years)} \]
Coupled modelling – Comparison Coarse mesh / Refined mesh

Deviatoric strains
• Localization study : Acoustic tensor determinant
• Mesh dependency of the results for classical FE
• Non-uniqueness of the results in both cases

The numerical modelling of strain localization with classical FE is not adequate.

We need another numerical model to fix this mesh dependency problem!
Outline:

- Introduction
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- Numerical models
- Numerical application
- Conclusions
Numerical models

• Classical FE formulation: mesh dependency

• Different regularization methods

  Gradient plasticity

  Non-local approach

  Microstructure continuum
    Cosserat model
    Second gradient local model

Mainly for monophasic materials!
In second gradient model, the continuum is enriched with microstructure effects. The kinematics include therefore the classical one but also microkinematics (See Germain 1973, Toupin 1962, Mindlin 1964).

Let us define first the classical kinematics:

- \( u_i \) is the (macro) displacement field
- \( F_{ij} \) is the macro displacement gradient which means:
  \[
  F_{ij} = \frac{\partial u_i}{\partial x_j}
  \]
- \( D_{ij} \) is the macro strain:
  \[
  D_{ij} = \frac{1}{2}(F_{ij} + F_{ji})
  \]
- \( R_{ij} \) is the macro rotation:
  \[
  R_{ij} = \frac{1}{2}(F_{ij} - F_{ji})
  \]
Enrichment of the kinematics:

The continuum is enriched with microstructure effects.

Macro-kinematics + micro-kinematics

Macro $\Omega$:

$$F_{ij} = \frac{\partial u_i}{\partial x_j} = D_{ij} + R_{ij}$$

Micro $\Omega^m$:

$$f_{ij} = \frac{\partial u_i^m}{\partial x_j} = d_{ij}^m + r_{ij}^m$$
Here is the enrichment:

- $f_{ij}$ is the microkinematic gradient.
- $d_{ij}$ is the microstrain:
  \[ d_{ij} = \frac{1}{2}(f_{ij} + f_{ji}) \]
- $r_{ij}$ is the microrotation:
  \[ r_{ij} = \frac{1}{2}(f_{ij} - f_{ji}) \]
- $h_{ijk}$ is the (micro) second gradient:
  \[ h_{ijk} = \frac{\partial f_{ij}}{\partial x_k} \]
• The internal virtual work (Germain, 1973)

\[ W^{*i} = \int_{\Omega} w^{*} \, dv = \int_{\Omega} (\sigma_{ij} D^{*}_{ij} + \tau_{ij} (f^{*}_{ij} - F_{ij}^{*}) + \chi_{ijk} h^{*}_{ijk}) \, dv \]

• The external virtual work (simplified)

\[ W^{*e} = \int_{\Omega} G_{i} u_{i}^{*} \, dv + \int_{\partial\Omega} (t_{i} u_{i}^{*} + T_{ij} f_{ij}^{*}) \, ds \]

• The virtual work equations can be extended to large strain problems
Numerical models

- **Balance equations**

\[
\frac{\partial (\sigma_{ij} - \tau_{ij})}{\partial x_j} + G_i = 0
\]

\[
\frac{\partial \chi_{ijk}}{\partial x_k} - \tau_{ij} = 0
\]

- **Boundary conditions**

\[
(\sigma_{ij} - \tau_{ij})n_j = t_i
\]

\[
\chi_{ijk}n_k = T_{ij}
\]

written in the current configuration

Three constitutive equations needed!
Local second gradient models: we add the kinematical constraint (Chambon et al., 1998; Matsushima et al., 2002)

\[ f_{ij} = F_{ij} \]

this implies:

\[ f_{ij} = \frac{\partial u_i}{\partial x_j} \]

the virtual work equation reads

\[
\int_{\Omega} \left( \sigma_{ij} D_{ij}^* + \chi_{ijk} \frac{\partial^2 u_i^*}{\partial x_j \partial x_k} \right) \, dv = \int_{\Omega} G_i u_i^* \, dv + \int_{\partial \Omega} \left( p_i u_i^* + P_i D u_i^* \right) \, ds
\]
Numerical models

- Local second gradient models

Balance equations

\[ \frac{\partial \sigma_{ij}}{\partial x_j} - \frac{\partial^2 \chi_{ijk}}{\partial x_j \partial x_k} + G_i = 0 \]

Boundary conditions

\[ \sigma_{ij} n_j - n_k n_j D\chi_{ijk} - \frac{D\chi_{ijk}}{Dx_k} n_j - \frac{D\chi_{ijk}}{Dx_j} n_k + \frac{Dn_l}{Dx_l} \chi_{ijk} n_j n_k - \frac{Dn_j}{Dx_k} \chi_{ijk} = p_i \]

\[ \chi_{ijk} n_j n_k = P_i \]
How do we introduce an internal length scale in second grade model?

Let’s take a simple example of a 1D-bar in traction:

\[ d\sigma = A_1 \, du' \text{ if } u' < e_{lim} \]
\[ d\sigma = A_2 \, du' \text{ if } u' > e_{lim} \]
\[ d\sigma = 0 \, du' \text{ if } u' > e_{lim} \left( \frac{A_1 + A_2}{A_2} \right) \]

\[ d\chi = B \, du'' \]
Numerical models

General differential equation of the 1D problem

\[
\frac{\partial \sigma_{ij}}{\partial x_j} - \frac{\partial^2 \chi_{ijk}}{\partial x_j \partial x_k} + G_i = 0 \quad \rightarrow \quad \frac{\partial \sigma_{11}}{\partial x} - \frac{\partial^2 \chi_{111}}{\partial x^2} = 0
\]

After two integrations, we obtain:

\[
A \cdot u - B u'' = N_1 x + AK
\]

Where \( N_1 = \sigma - \chi' = \text{Cst} \) and \( K = \text{Cst} \),

\( A = A_1 \) if \( u' < e_{lim} \)

\( A = A_2 \) if \( u' > e_{lim} \)
General differential equation of the problem \[ A \cdot u - B \cdot u'' = N_1 \cdot x + AK \]

General solution of the problem

\[ u = \left( \frac{N_1}{A_1} \right) x + K + \alpha \cdot \cosh(\omega x) + \beta \cdot \sinh(\omega x) ; \quad \omega^2 = \frac{A_1}{B} > 0 \]

if \( u' < e_{\text{lim}} \)

\[ u = \left( \frac{N_1}{A_1} \right) x + K + \alpha \cdot \cos(\eta x) + \beta \cdot \sin(\eta x) ; \quad -\eta^2 = \frac{A_2}{B} < 0 \]

if \( u' > e_{\text{lim}} \)
Let's take another example: thick-walled cylinder problem (elastic second gradient model)

Balance equation

\[ \partial_r (r \sigma_{rr}) - \sigma_{\theta \theta} + \frac{1}{r} \partial_r (r (\chi_{\theta \theta r} + \chi_{r \theta \theta} + \chi_{\theta r \theta})) - \partial_r^2 (r \chi_{\theta r r}) = 0 \]

General differential equation of the problem

\[ (\lambda + 2\mu) r \partial_r v - B r \partial_r \left( \frac{1}{r} \partial_r (r \partial_r v) \right) = 0 \]

\[ v = \frac{1}{r} \partial_r (ru) \]

General solution

\[ u = C_1 B^l \left( 1, \frac{r}{\alpha} \right) + C_2 B^K \left( 1, \frac{r}{\alpha} \right) + C_3 r + \frac{C_4}{r} \]

\[ \alpha = \frac{B}{\sqrt{\lambda + 2\mu}} \]
Finite element formulation of a second grade model

- **Local second gradient model**: additional assumption \( v_{ij}^* = F_{ij}^* \)

\[
\int_{\Omega} \left( \sigma_{ij} \frac{\partial u_i^*}{\partial x_j} + \sum_{ijk} \frac{\partial^2 u_i^*}{\partial x_j \partial x_k} \right) d\Omega = W_{ext}^*
\]

**Local quantities**

Introduction of Lagrange multiplier field:

\[
\int_{\Omega} \left( \sigma_{ij} \frac{\partial u_i^*}{\partial x_j} + \sum_{ijk} \frac{\partial v_{ij}^*}{\partial x_k} \right) d\Omega - \int_{\Omega} \lambda_{ij} \left( \frac{\partial u_i^*}{\partial x_j} - v_{ij}^* \right) d\Omega = W_{ext}^*
\]

\[
\int_{\Omega} \lambda_{ij}^* \left( \frac{\partial u_i}{\partial x_j} - v_{ij} \right) d\Omega = 0
\]
Local Second gradient Finite element

- $u_i$
- $v_{ij}$
- $\lambda_{ij}$
Numerical models

Example n°1 (again)

- **Biaxial compression test**

  **Smooth and rigid boundary**

  **Bottom-left defect**

  **Strain rate : 0.18% / hour**

  **No lateral confinement**

  **Globally drained (upper and lower drainage)**
Numerical models

- First gradient law:

  **Linear elasticity:** $E_0$ and $\nu_0$

  **Drucker Prager criterion:**
  $$F = \sqrt{\frac{3}{2}} II_{\hat{\sigma}} + m \left( I_\sigma - \frac{3c}{\tan \phi} \right) = 0$$

  $$m = \frac{2 \sin \phi}{3 - \sin \phi} \quad c = c_0 f(\gamma^p)$$

  **Associated softening plasticity (decrease of cohesion):**

  $$f(\gamma^p) = \left( 1 - (1 - \alpha) \frac{\gamma^p}{\gamma_R^p} \right)^2 \text{ si } 0 < \gamma^p < \gamma_R^p$$

  $$= \alpha^2 \text{ si } \gamma^p \geq \gamma_R^p$$

  $E = 5800 \text{ MPa}$  \quad $\phi = 25^\circ$  \quad $c_0 = 1 \text{ MPa}$

  $\nu = 0,3$  \quad $\psi = 25^\circ$  \quad $\alpha = 0,01$

  $\gamma_R = 0,015$
Numerical models

- **Second gradient law**: Linear relationship deduced from Mindlin

\[
\begin{bmatrix}
\dot{\Sigma}_{111} \\
\dot{\Sigma}_{112} \\
\dot{\Sigma}_{121} \\
\dot{\Sigma}_{122} \\
\dot{\Sigma}_{211} \\
\dot{\Sigma}_{212} \\
\dot{\Sigma}_{221} \\
\dot{\Sigma}_{222}
\end{bmatrix}
= 
\begin{bmatrix}
D & 0 & 0 & 0 & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\
0 & \frac{D}{2} & \frac{D}{2} & 0 & -\frac{D}{2} & 0 & 0 & \frac{D}{2} \\
0 & \frac{D}{2} & \frac{D}{2} & 0 & -\frac{D}{2} & 0 & 0 & \frac{D}{2} \\
0 & 0 & 0 & D & 0 & -\frac{D}{2} & -\frac{D}{2} & 0 \\
0 & -\frac{D}{2} & -\frac{D}{2} & 0 & D & 0 & 0 & 0 \\
\frac{D}{2} & 0 & 0 & -\frac{D}{2} & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\
\frac{D}{2} & 0 & 0 & -\frac{D}{2} & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\
0 & \frac{D}{2} & \frac{D}{2} & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\frac{\partial \psi_{11}}{\partial x_1} \\
\frac{\partial \psi_{12}}{\partial x_1} \\
\frac{\partial \psi_{12}}{\partial x_2} \\
\frac{\partial \psi_{21}}{\partial x_1} \\
\frac{\partial \psi_{21}}{\partial x_2} \\
\frac{\partial \psi_{22}}{\partial x_1} \\
\frac{\partial \psi_{22}}{\partial x_2}
\end{bmatrix}
\]

\( D = 20 \text{ kN} \)
First modelling: no HM coupling (no overpressure)

Bifurcation directions

(Regularization : Second gradient)
First modelling: no HM coupling (no overpressure)

Plastic loading point

(Regularization : Second gradient)
**First modelling: no HM coupling (no overpressure)**

*Velocity field*  

(Regularization: Second gradient)
Initiation of localization (Directional research – Chambon et al., 2001)
Initiation of localization (Directional research)

(Regularization : Second gradient)

Non uniqueness of the solution
Initiation of localization (Directional research)

(Regularization: Second gradient)

Non uniqueness of the solution
Numerical models

Localization mode switching (Bésuelle et al., 2006)

Non uniqueness of the solution
Initiation of localization (Directional research)

(Regularization : Second gradient)

Non uniqueness of the solution

Sieffert et al., 2009
Our goal is to extend the second gradient formulation for multiphysics conditions. In the following, we focus on the hydromechanical model but the same procedure can be applied for TM, THM or THMC problems.

- **Main assumptions**
  - Quasi static motion
  - Fully saturated
  - Incompressible solid grains

- **Aims**
  - Equations written in the spatial configuration
  - Full Newton Raphson method
• **Classical poromechanics field equations**

*Saturated porous medium*

**Balance of linear momentum for the mixture**

\[
\int_{\Omega} \sigma_{ij} \dot{\varepsilon}_{ij}^* d\Omega = \int_{\Omega} \rho_{mix} g_i u_i^* d\Omega + \int_{\Gamma} \bar{t}_i u_i^* d\Gamma
\]

**Boundary condition**  \[ \sigma_{ij} n_j = \bar{t}_i \]

**Terzaghi’s postulate**  \[ \sigma_{ij} = \sigma_{ij}' - p \delta_{ij} \]
• **Classical poromechanics field equations**

**Fluid mass balance**

\[
\int_{\Omega} \dot{M} p^* - m_i \frac{\partial p^*}{\partial x_i} d\Omega = \int_{\Omega} Q p^* d\Omega + \int_{\Gamma} \bar{q} p^* d\Gamma
\]

**Boundary condition**

\[
\bar{q} = m_i n_i
\]

**Darcy’s law**

\[
m_i = -\rho_w \frac{k}{\mu} \left( \frac{\partial p}{\partial x_i} + \rho_w g_i \right)
\]

**Storage law**

\[
\dot{M} = \rho_w \frac{\dot{p}}{k^w} \phi + \rho_w \frac{\dot{\Omega}}{\Omega}
\]
• Classical poromechanics field equations

Balance of momentum for the fluid phase

\[ \frac{\partial p^t}{\partial x_i^t} + F_{i}^{S/W,t} + g^{w,t} g_i = 0 \]

Viscous drag force:

\[ F_{i}^{S/W,t} = \frac{g^{w,t} \phi^t g}{K} V_i^{W/S,t} \]

Mass balance equation for the solid

\[ \frac{\partial (\rho_s (1 - \phi^t) \Omega^t)}{\partial t} = 0 \]
• Coupled local second gradient model

✓ Second gradient effects are assumed only for solid phase

✓ For the mixture, there are stresses which obey the Terzaghi postulate and double stresses which are only the one of the solid phase

✓ Boundary conditions for the mixture are enriched
**Numerical models**

- **Coupled local second gradient model**

\[
\int_{\Omega} \left( \sigma_{ij} \frac{\partial u_i^*}{\partial x_j} + \Sigma_{ijk} \frac{\partial^2 u_i^*}{\partial x_j \partial x_k} \right) d\Omega = \int_{\Omega} \rho_{\text{mix}} g_i u_i^* d\Omega + \int_{\Gamma} t_i u_i^* + \bar{T}_i Du_i^* d\Gamma
\]

\[
\int_{\Omega} \dot{M} p^* - m_i \frac{\partial p^*}{\partial x_i} d\Omega = \int_{\Omega} Q p^* d\Omega + \int_{\Gamma} \bar{q} p^* d\Gamma
\]
• **Coupled local second gradient model**

\[
\int_{\Omega} \left( \sigma_{ij} \frac{\partial u_i^*}{\partial x_j} + \sum_{ijk} \frac{\partial v_{ij}^*}{\partial x_k} \right) d\Omega - \int_{\Omega} \lambda_{ij} \left( \frac{\partial u_i^*}{\partial x_j} - v_{ij}^* \right) d\Omega = \\
\int_{\Omega} \rho_{mix} g_i u_i^* d\Omega + \int_{\Gamma} \bar{t}_i u_i^* + \bar{T}_i D u_i^* d\Gamma
\]

\[
\int_{\Omega} \dot{M} p^* - m_i \frac{\partial p^*}{\partial x_i} d\Omega = \int_{\Omega} Q p^* d\Omega + \int_{\Gamma} \bar{q} p^* d\Gamma
\]

\[
\int_{\Omega} \lambda_{ij}^* \left( \frac{\partial u_i}{\partial x_j} - v_{ij} \right) d\Omega = 0
\]
Finite element formulation of the coupled local second gradient model

✓ Equations are assumed to be met at time $t$

✓ We are looking for the values of the different fields at time: $t + \Delta t = \tau_1$

✓ using a full Newton Raphson method and an implicit scheme for the rate:

$$\dot{p}^{t+\Delta t} = \frac{p^{t+\Delta t} - p^t}{\Delta t}$$
• **Field equations at time** $t + \Delta t$

\[
\int_{\Omega^1} \left( \sigma_{ij}^{1} \frac{\partial u_i^*}{\partial x_j^1} + \Sigma_{ijk}^{1} \frac{\partial v_{ij}^*}{\partial x_k^1} \right) d\Omega^1 - \int_{\Omega^1} \lambda_{ij}^{1} \left( \frac{\partial u_i^*}{\partial x_j^1} - v_{ij}^* \right) d\Omega^1 -
\int_{\Omega^1} \left( q^s (1 - \phi^1) + q^w,\phi^1 \right) g_i u_i^* d\Omega^1 - \int_{\Gamma^1} \left( t_i u_i^* + T_i v_{ik}^* n_k^1 \right) d\Gamma^1 = R^1,
\]

\[
\int_{\Omega^1} \lambda_{ij}^{1} \left( \frac{\partial u_i^*}{\partial x_j^1} - v_{ij}^* \right) d\Omega^1 = S^1,
\]

\[
\int_{\Omega^1} \left( \dot{M}^1 p^* - m_i^1 \frac{\partial p^*}{\partial x_i^1} \right) d\Omega^1 - \int_{\Omega^1} Q^1 p^* d\Omega^1 + \int_{\Gamma_q^1} q^1 p^* d\Gamma^1 = W^1.
\]

$R$, $S$ and $W$ : Residuals of the balance equations
• **Linearization of field equations**

**Auxiliary linear problem**

\[
\int_{\Omega} \left[ U^{*}_{(x,y)} \right]^T \left[ E \right] \left[ dU_{(x,y)} \right] d\Omega = -R - S - W
\]

**R, S and W : Residuals of the balance equations**

\[
\left[ dU_{(x,y)} \right] = \left[ \frac{\partial du_1}{\partial x_1} \frac{\partial du_1}{\partial x_2} \frac{\partial du_2}{\partial x_1} \frac{\partial du_2}{\partial x_2} du_1 du_2 \frac{\partial dp}{\partial x_1} \frac{\partial dp}{\partial x_2} dp \right]
\]

\[
\left[ \begin{array}{c}
\frac{\partial dv_{11}}{\partial x_1} \frac{\partial dv_{11}}{\partial x_2} \frac{\partial dv_{12}}{\partial x_1} \cdots \frac{\partial dv_{22}}{\partial x_2} dv_{11} \cdots dv_{22} d\lambda_{11} \cdots d\lambda_{22}
\end{array} \right]
\]
Numerical models

\[
[E] = \begin{bmatrix}
E_1^{(4 \times 4)} & 0^{(4 \times 2)} & K_{WM}^{(4 \times 3)} & 0^{(4 \times 8)} & 0^{(4 \times 4)} & -I^{(4 \times 4)} \\
G_1^{(2 \times 4)} & 0^{(2 \times 2)} & G_2^{(2 \times 3)} & 0^{(2 \times 8)} & 0^{(2 \times 4)} & 0^{(2 \times 4)} \\
K_{MW}^{(3 \times 4)} & 0^{(3 \times 2)} & K_{WW}^{(3 \times 3)} & 0^{(3 \times 8)} & 0^{(3 \times 4)} & 0^{(3 \times 4)} \\
E_2^{(8 \times 4)} & 0^{(8 \times 2)} & 0^{(8 \times 3)} & D^{(8 \times 8)} & 0^{(8 \times 4)} & 0^{(8 \times 4)} \\
E_3^{(4 \times 4)} & 0^{(4 \times 2)} & 0^{(4 \times 3)} & 0^{(4 \times 8)} & 0^{(4 \times 4)} & I^{(4 \times 4)} \\
E_4^{(4 \times 4)} & 0^{(4 \times 2)} & 0^{(4 \times 3)} & 0^{(4 \times 8)} & -I^{(4 \times 4)} & 0^{(4 \times 4)}
\end{bmatrix}
\]

*E1, E2, E3, E4 and D*: see monophasic local sec. Gradient model

*G1 and G2*: related to gravity volume force

*K_{WW}*: Classical flow matrix

*K_{MW} and K_{WM}*: Coupling terms including large strain effect
Isoparametric Finite Element:

8 nodes for macro-displacement and pressure field
4 nodes for microkinetic gradient field
1 node for Lagrange multipliers field
FE element discretization of linear auxiliary problem

\[
\begin{bmatrix} U_{\text{node}}^* \end{bmatrix}^T \int_{-1}^{1} \int_{-1}^{1} [B]^T [T]^T [E][T][B] \det J \, d\xi \, d\eta \, [dU_{\text{node}}] \equiv \\
\begin{bmatrix} U_{\text{node}}^* \end{bmatrix}^T [k][dU_{\text{node}}]
\]

Local stiffness matrix

\[-R - S - W = P_{\text{ext}}^* - \begin{bmatrix} U_{\text{node}}^* \end{bmatrix}^T \int_{-1}^{1} \int_{-1}^{1} [B]^T [T]^T [\sigma] \det J \, d\xi \, d\eta \equiv \\
\begin{bmatrix} U_{\text{node}}^* \end{bmatrix}^T [f_{HE}]
\]

Elementary out of balance forces
Example n°1 (last time)

- **Biaxial compression test**

  *Smooth and rigid boundary*

  *Bottom-left defect*

  *Strain rate: 0.18% / hour*

  *No lateral confinement*

  *Globally drained (upper and lower drainage)*
Numerical models

- **Second gradient law**: Linear relationship deduced from Mindlin

\[
\begin{bmatrix}
\tilde{\Sigma}_{111} \\
\tilde{\Sigma}_{112} \\
\tilde{\Sigma}_{121} \\
\tilde{\Sigma}_{122} \\
\tilde{\Sigma}_{211} \\
\tilde{\Sigma}_{212} \\
\tilde{\Sigma}_{221} \\
\tilde{\Sigma}_{222}
\end{bmatrix}
= 
\begin{bmatrix}
D & 0 & 0 & 0 & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\
0 & \frac{D}{2} & \frac{D}{2} & 0 & -\frac{D}{2} & 0 & 0 & \frac{D}{2} \\
0 & \frac{D}{2} & \frac{D}{2} & 0 & -\frac{D}{2} & 0 & 0 & \frac{D}{2} \\
0 & 0 & 0 & D & 0 & -\frac{D}{2} & -\frac{D}{2} & 0 \\
0 & -\frac{D}{2} & -\frac{D}{2} & 0 & D & 0 & 0 & 0 \\
\frac{D}{2} & 0 & 0 & -\frac{D}{2} & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\
\frac{D}{2} & 0 & 0 & -\frac{D}{2} & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\
0 & \frac{D}{2} & \frac{D}{2} & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\frac{\partial \psi_{11}}{\partial x_1} \\
\frac{\partial \psi_{11}}{\partial x_2} \\
\frac{\partial \psi_{12}}{\partial x_1} \\
\frac{\partial \psi_{12}}{\partial x_2} \\
\frac{\partial \psi_{21}}{\partial x_1} \\
\frac{\partial \psi_{21}}{\partial x_2} \\
\frac{\partial \psi_{22}}{\partial x_1} \\
\frac{\partial \psi_{22}}{\partial x_2}
\end{bmatrix}
\]

\(D = 20 \text{ kN}\)

- **Flow model parameters**

\(\kappa = 10^{-19} / 10^{-12} \text{ m}^2\)

\(\rho_w = 1000 \text{ kg/m}^3\)

\(\phi = 0.15\)

\(k_w = 5 \times 10^{-10} \text{ Pa}^{-1}\)

\(\mu_w = 0.001 \text{ Pa.s}\)
Second modelling: HM coupling

• Equivalent strain after 0.2% of axial strain ($\kappa = 10^{-12} \text{ m}^2$)

(20 x 10)  (30 x 15)  (40 x 20)
• Plastic loading point after 0.2 % of axial strain ($\kappa = 10^{-12} \, m^2$)
• Fluid flow after 0.2 % of axial strain ($\kappa = 10^{-12} \, m^2$)
• *Load-displacement curve* \( (\kappa = 10^{-12} \, m^2) \)
Second modelling: HM coupling

- Load-displacement curve ($\kappa = 10^{-19} \text{ m}^2$)

'Undrained' behaviour
For $\kappa = 10^{-19} \text{ m}^2$, the behaviour is undrained, we recover the experimental observation showing that for dilatant material, no localization is possible before cavitation.
Random initialization (coupled problem)

\[ q = \sigma_1 - \sigma_3 \text{ [MPa]} \]

Homogeneous solution

Localized solution (random initialization)
Random initialization (coupled problem)

\[ q = \sigma_1 - \sigma_3 \text{ [MPa]} \]

Deviatoric strain increment
Numerical models

Random initialization (coupled problem)

Deviatoric strain increment

Decrease of $q = \text{disappearance of a shear band}$
Coupled modelling – Comparison Coarse mesh - Refined mesh

Classical FE formulation

Deviatoric strains
Coupled modelling – Comparison Coarse mesh - Refined mesh

Coupled second gradient FE formulation

Deyiatomic strains
Outline:

- Introduction
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- Numerical models
- Numerical application
- Conclusions
Example of EDZ around a cavity

**Long-term management of radioactive wastes**

- **Deep geological disposal**
  - Repository in deep geological media with good confining properties
  - (Low permeability $K<10^{-12} \text{ m/s}$)

- **Intermediate** (long-lived) & high activity wastes

- Underground structures
  - = network of galleries

- **Disposal facility of Cigéo project in France**
  - (Labalette et al., 2013)
Example of EDZ around a cavity

Repository phases

**Construction**
- Excavation

**Maintenance**
- Ventilation

**Repository**
- Sealing

**Long term**
- Corrosion, heat generation

Repository phases over time:
- Construction
- Maintenance
- Repository
- Long term

Type C wastes (Andra, 2005)
Excavation Damaged Zone (EDZ)

Fracturing & permeability increase (several orders of magnitude)

Opalinus clay in Switzerland (Bossart et al., 2002)
Example of EDZ around a cavity

**Callovo-Oxfordian claystone (COx)**

Sedimentary clay rock (France).

- Underground research laboratory
- Feasibility of a safe repository
- France (Meuse / Haute-Marne, Bure)
Example of EDZ around a cavity

- Fracturing

Anisotropies:
- stress: $\sigma_H > \sigma_h \sim \sigma_v$
- material: HM cross-anisotropy.

Issues:
Prediction of the fracturing.
Effect of anisotropies?
Permeability evolution & relation to fractures?

(Armand et al., 2014)
Example of EDZ around a cavity

**Constitutive models for COx**

- **Mechanical law - 1st gradient model**

  Isotropic elasto-plastic internal friction model
  
  Non-associated plasticity, Van Eeckelen yield surface:
  
  \[ F = II_{\sigma} - m \left( I_{\sigma'} + \frac{3c}{\tan \varphi_C} \right) \]

\[ F = 0 \]

φ hardening / c softening

\[ c = c_0 + \left( c_f - c_0 \right) \varepsilon_{eq}^p \]

→ Strain localisation

- **Hydraulic law**

  Fluid mass flow (advection, Darcy):

  \[ f_{w,i} = -\rho_w \frac{k_{w,i} k_{r,w}}{\mu_w} \left( \frac{\partial p_w}{\partial x_j} + \rho_w g_j \right) \]

  Water retention and permeability curves (Mualem - Van Genuchten's model)
Example of EDZ around a cavity

**Gallery excavation modelling**

- **Numerical model**
  HM modelling in 2D plane strain state
  Gallery radius = 2.3 m

- **Gallery in COx // $\sigma_H$**

**Effect of stress anisotropy**

Anisotropic stress state
- $p_{w,0} = 4.5$ [MPa]
- $\sigma_{x,0} = \sigma_H = 1.3 \sigma_v = 15.6$ [MPa]
- $\sigma_{y,0} = \sigma_v = 12$ [MPa]
- $\sigma_{z,0} = \sigma_H = 12$ [MPa]

- **Excavation**

[Introduction Theory Models Application Conclusions]
Example of EDZ around a cavity

- Localisation zone

Incompressible solid grains, $b=1$

\[ \sigma_r / \sigma_r,0 = 0.4 \]
\[ \sigma_r / \sigma_r,0 = 0.2 \]
\[ \sigma_r / \sigma_r,0 = 0.0 \]
\[ \sigma / \sigma_0 = 0.00 \]
\[ \sigma / \sigma_0 = 0.00 \]

Total deviatoric strain

Plasticity

\[ \hat{\varepsilon}_{eq} = \sqrt{\frac{2}{3} \hat{\varepsilon}_{ij} \hat{\varepsilon}_{ij}} \]

\[ \hat{\varepsilon} \quad \hat{\varepsilon} \quad \hat{\varepsilon} \]

1000 days

End of excavation

For an isotropic mechanical behaviour, the appearance and shape of the strain localisation are mainly due to mechanical effects linked to the anisotropic stress state.
Example of EDZ around a cavity

- Gallery air ventilation:

Water phases equilibrium at gallery wall (Kelvin’s law)

\[ RH = \frac{p_v}{p_{v,0}} = \exp\left(\frac{-p_c M_v}{RT \rho_w}\right) \]

Compressibility of the solid grains: \( b = 0.6 \)

No ventilation

\[ p_w = \rho_{atm} \text{ [MPa]} \]

Ventilation

\[ p_w = -30.7 \text{ [MPa]} \]

Introduction

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Example of EDZ around a cavity

- Convergence:
  Important during the excavation
  Anisotropic convergence
  Influence of the ventilation
  Experimental results (GED - Andra’s URL)
  No strain localisation

![Graph showing convergence over time](image)

- Numerical, RH=100%, no ventilation
- Numerical, RH=80%, ventilation
- Experimental, GED
- Numerical, no strain localisation RH=80%, ventilation
Large-scale experiment of gallery ventilation (SDZ)

Characterise the effect of gallery ventilation on the hydraulic transfer around it.

→ drainage / desaturation
→ exchange at gallery wall

Introduction  Theory  Models  Application  Conclusions
Permeability variation in fractured zone

HM coupling in the EDZ.

Saturated permeability in boreholes

Fracture and rock matrix permeabilities

- Capture $k_w$ evolution
- Relation to fractures
Example of EDZ around a cavity

Evolution of intrinsic water permeability

Various approaches: deformation, damage, cracks…

- Relation to deformation

Volumetric effects = increase of porous space
(Kozeny-Carman)

\[ k_w = k_{w,0} \left(1 - \phi_0\right)^{\varepsilon_n} \phi_0^{\varepsilon_2} \frac{\phi_0^{\varepsilon_2}}{(1 - \phi)^{\varepsilon_n}} \]

\[ \varepsilon_v = \frac{\varepsilon_{ii}}{3} \]

- Fracture permeability

Cubic law for parallel-plate approach
(Witherspoon 1980; Snow 1969, Olivella and Alonso 2008)

\[ k_w = \frac{b^3}{12B} \]

\[ b = b_0 + B \left( \varepsilon^n - \varepsilon_0^n \right) \]

\[ k_w = k_{w,0} \left(1 + A \left( \varepsilon^n - \varepsilon_0^n \right) \right)^3 \]

Localised deformation
Fracture initiation

- Empirical law

Related to strain localisation effect
Permeability variation threshold

\[ k_{w,ij} = k_{w,ij,0} \left(1 + \beta_{per} \left( YI - YI^{thr} \right) \right) \]

\[ YI = \frac{\Pi_{\sigma}}{\Pi_{\rho}^p} \]
Modelling of excavation and SDZ experiment

**HM coupling in EDZ**

- Gallery excavation

SDZ → GED gallery // $\sigma_h$

Anisotropic $\sigma_{ij,0}$ and material

→ Localisation zone dominated by stress anisotropy

- Intrinsic permeability evolution

\[
\frac{k_{w,ij}}{k_{w,ij,0}} = \left(1 + \beta \left( YI - YI^{thr} \right) \right)^3
\]

$YI^{thr} = 0.95$

Cross-sections

Plastic strain and a part of the elastic one

$\rightarrow$ EDZ extension + $k_w$ increase

**Introduction**

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Modelling of the SDZ experiment

- Water pressure in the cavity air

\[ p^\text{air}_w = \frac{\rho_w RT}{M_v} \ln(RH) + p_{\text{atm}} \]

\[ \rho^\text{air}_v = RH \rho_v^0 \]

Imposed at gallery wall through hydraulic boundary condition.

Excavation (RH=100%) \( \rightarrow \) Initiation phase \( \rightarrow \) Ventilation
Example of EDZ around a cavity

- Drainage / $p_w$ reproduction

Introduction  Theory  Models  Application  Conclusions

Oblique 45°

Horizonal

$\alpha_v = 10^{-3} \text{ m/s}$
Example of EDZ around a cavity

- Desaturation EDZ / \( w \) reproduction

Desaturation: overestimation in long term
Vapour transfer: \( \alpha_v = 10^{-3} \text{ m/s} \)

- Good reproduction at gallery wall

\[
w = \frac{M_w}{M_s}
\]
Outline:

- Introduction
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- Conclusions
Strain localization in shear band mode can be observed in most laboratory tests leading to rupture in geomaterials.

Complex localization patterns may be the result of specific geometrical or loading conditions.

The numerical modelling of strain localization with classical FE is not adequate. Enhanced models are needed for a robust modelling of the post peak behaviour.