Numerical modelling of multiphysics couplings and the strain localization

Collin F., P. Kotronis, B. Pardoen

P. Bésuelle, D. Caillerie, R. Chambon

ALERT Doctoral School (6th-8th Octobre 2016)

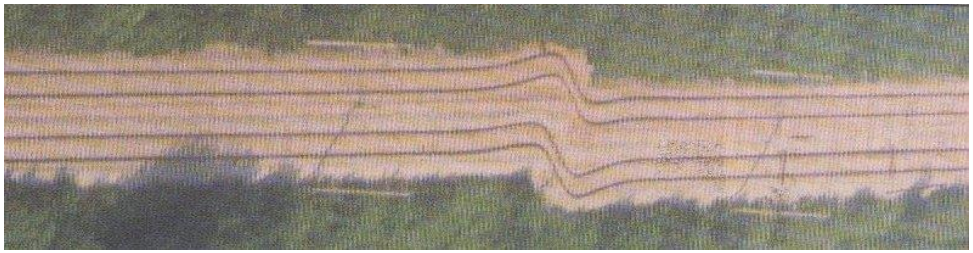
Failure in soils and rocks is almost always associated with fractures and/or shear bands developing in the geomaterial.

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

INTRODUCTION
In situ observation of shear banding

In situ observations of shear banding and/or faulting are made frequently at many scales



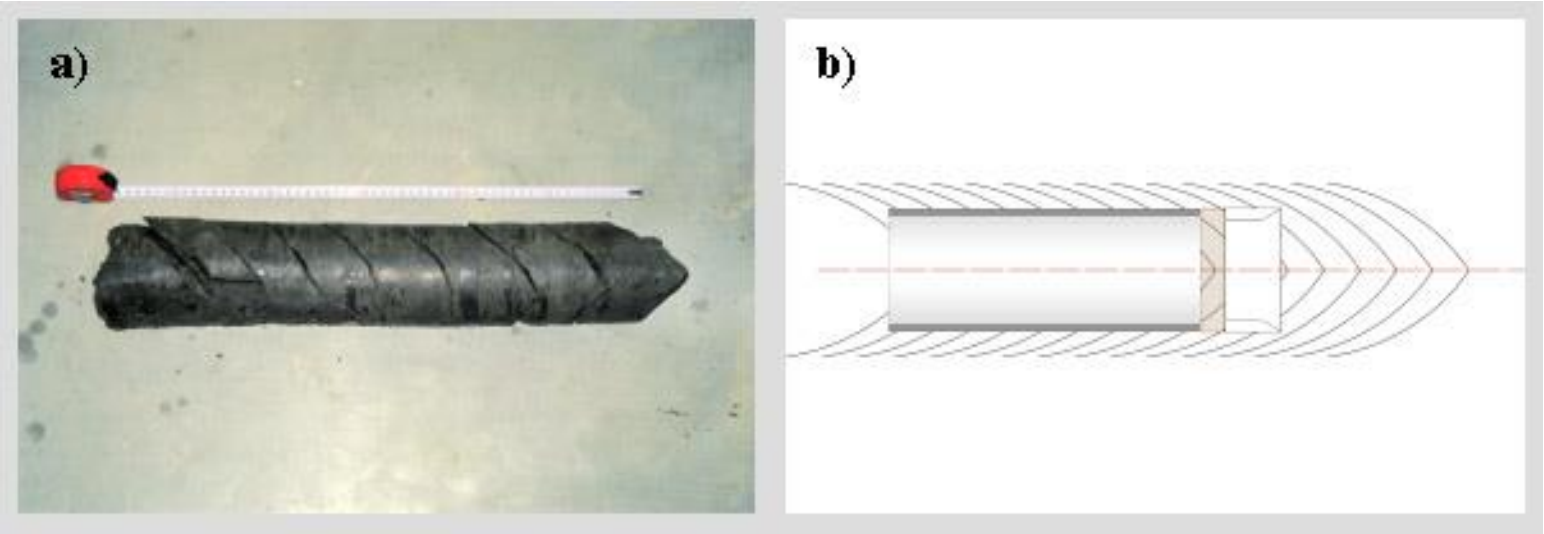
Large scale: railway tracks after an earthquake in Turkey

In situ observation of shear banding

Human-made slope along E42 exit road

Bierset (Belgium) 1998 – Courtesy C. Schroeder

Nuclear waste disposal



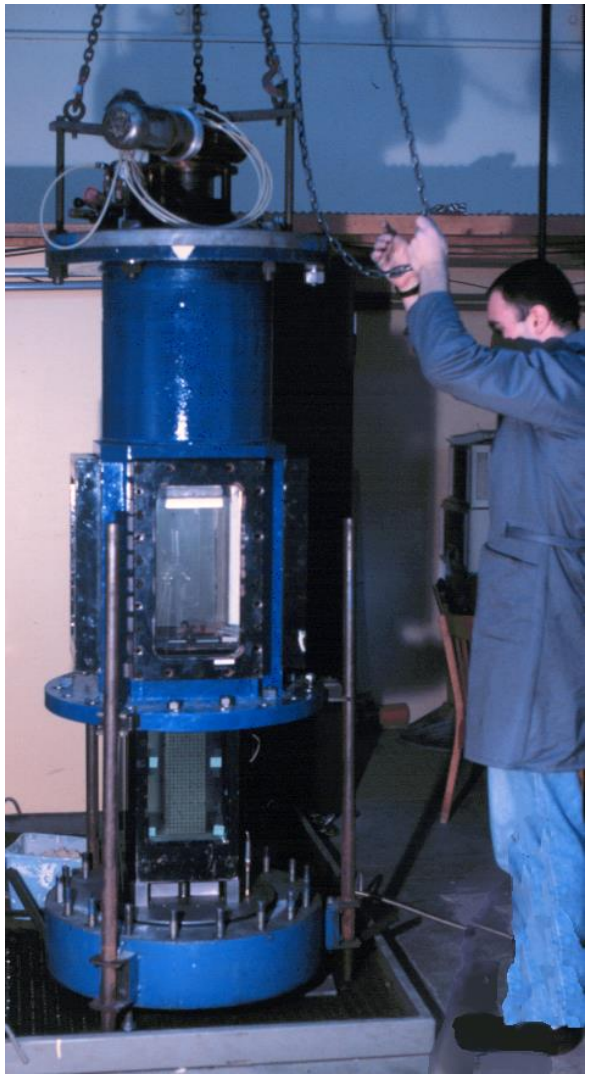
Fractures observed during the construction of the connecting gallery at the URL in Mol. Vertical cross section through the gallery showing the fracturation pattern around it, as deduced from the observations (from Alheid et al. 2005)

Experimental observations: triaxial test

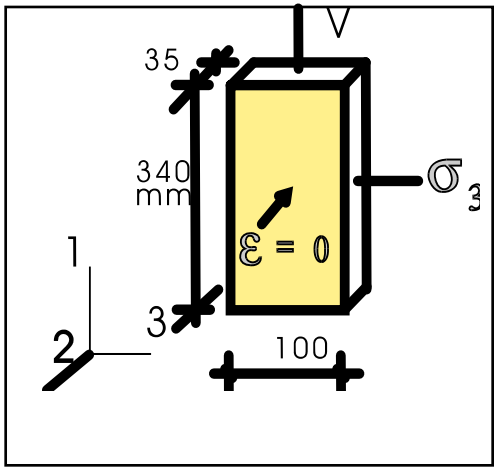
Localized rupture in sandstone samples under different confining pressures (Bésuelle et al., 2000)

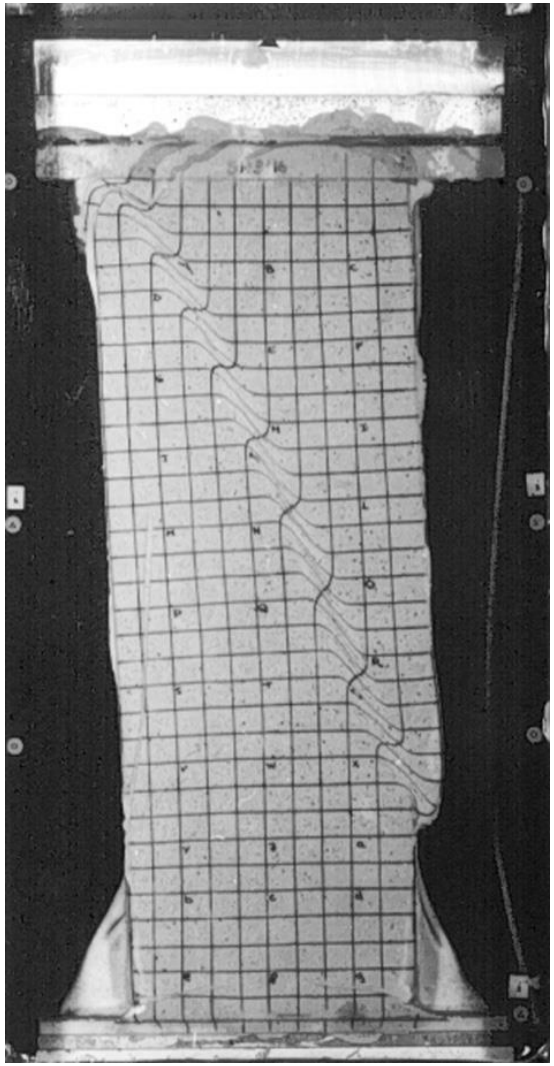
Experimental characterisation of the localisation phenomenon inside a Vosges sandstone in a triaxial cell
P. BESUELLE, J. DESRUES, S. RAYNAUD, International Journal of Rock Mechanics & Mining Sciences 37 (2000) p. 1223-1237

Experimental observations: biaxial test



Experimental
set-up
&
a typical test





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

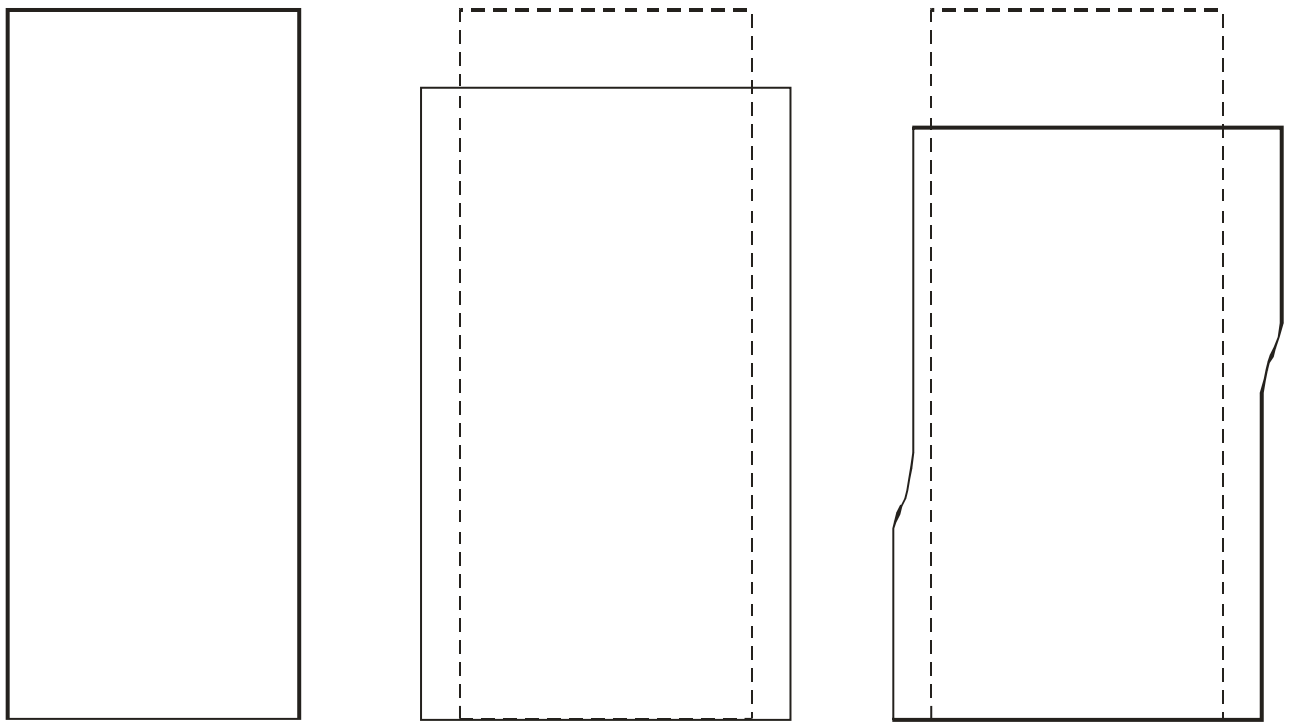
In geomaterials, the understanding of failure processes is more complex by the fact that soils and rocks are multiphase porous materials where different multiphysical processes take place.

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

Outline:

- *Introduction*
- *Theoretical tools*
- *Numerical models*
- *Numerical application*
- *Conclusions*

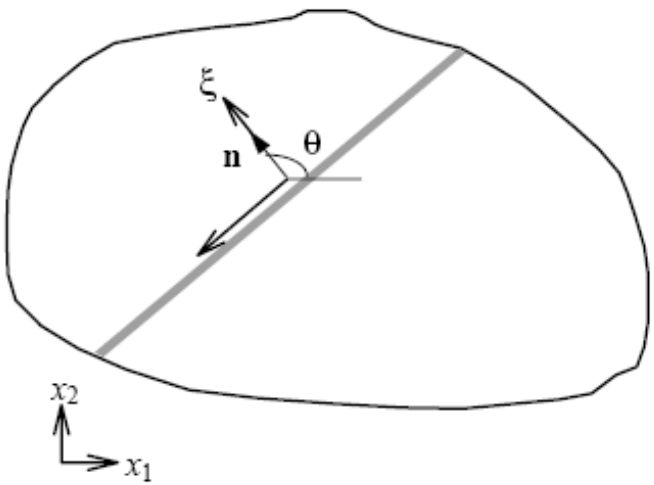
Experimental evidence:

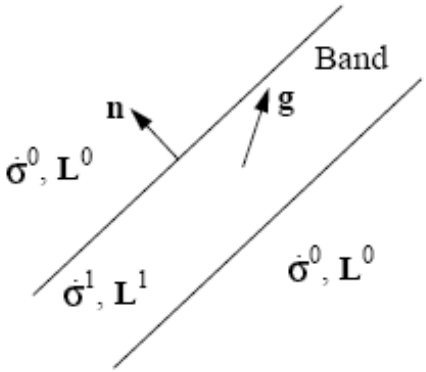


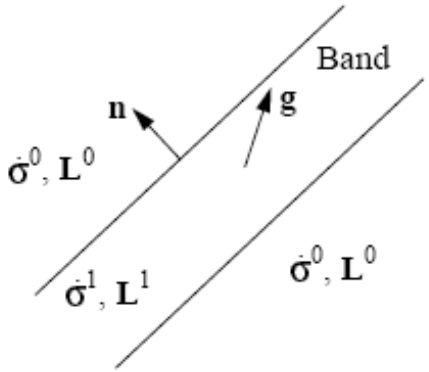
Initial state | Homogeneous strain field | Localized strain field

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.







$$L = \frac{1}{2}\left(\frac{\partial \dot{u}_i}{\partial x_j} + \frac{\partial \dot{u}_j}{\partial x_i}\right)$$

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

Kinematic condition: $L^1 = L^0 + \Delta L$

$$L^1 = L^0 + g \otimes n$$

Constitutive law: $\dot{\sigma} = C : L$

$$n\left(C^1 : (L^0 + g \otimes n) - C^0 : L^0\right) = 0$$

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

$$\det(nCn) \leq 0$$

Constitutive law in principal axis:

$$\begin{Bmatrix} \dot{\sigma}_{11} \\ \dot{\sigma}_{22} \\ \dot{\sigma}_{12} \end{Bmatrix} = \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{21} & C_{22} & 0 \\ 0 & 0 & 2G_{12} \end{bmatrix} \begin{Bmatrix} L_{11} \\ L_{22} \\ L_{12} \end{Bmatrix}$$

Static condition:

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

$$\begin{cases} \left(\dot{\sigma}_{11}^{1} - \dot{\sigma}_{11}^{0}\right) n_1 + \left(\dot{\sigma}_{12}^{1} - \dot{\sigma}_{12}^{0}\right) n_2 = 0 \\ \left(\dot{\sigma}_{21}^{1} - \dot{\sigma}_{21}^{0}\right) n_1 + \left(\dot{\sigma}_{22}^{1} - \dot{\sigma}_{22}^{0}\right) n_2 = 0 \end{cases}$$

Kinematic condition:

$$L_{ij}^{1} = L_{ij}^{0} + g_i n_j$$

Combining the three previous relationship yields:

If $C^1 = C^0 = C$:

$$\begin{cases} \left(C_{11} g_1 n_1 + C_{12} g_2 n_2\right) n_1 + G_{12}\left(g_1 n_2 + g_2 n_1\right) n_2 = 0 \\ G_{12}\left(g_1 n_2 + g_2 n_1\right) n_1 + \left(C_{21} g_1 n_1 + C_{22} g_2 n_2\right) n_2 = 0 \end{cases}$$

$$\begin{cases} \left(C_{11}n_1^{\ 2}+G_{12}n_2^{\ 2}\right)g_1+\left(C_{12}n_1n_2+G_{12}n_2n_1\right)g_2=0 \\ \left(C_{21}n_1n_2+G_{12}n_2n_1\right)g_1+\left(C_{22}n_2^{\ 2}+G_{12}n_1^{\ 2}\right)g_2=0 \end{cases}$$

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

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

$$n_1^{\ 4}\left(a_1\,z^4+a_3\,z^2+a_5\right)=0 \qquad z=\frac{n_2}{n_1}$$

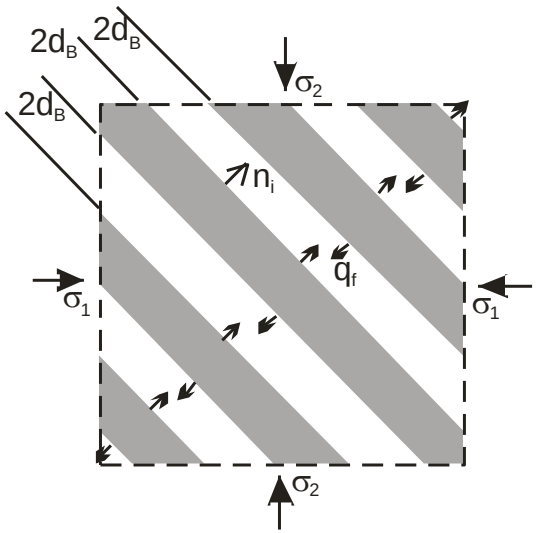
For a constitutive law written in cartesian axis:

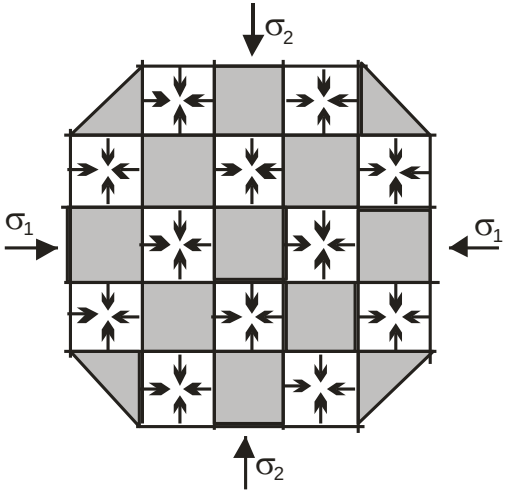
$$n_1^{\ 4}\left(a_1\,z^4+a_2\,z^3+a_3\,z^2+a_4\,z+a_5\right)=0$$

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* ν_0

Drucker Prager criterion :

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

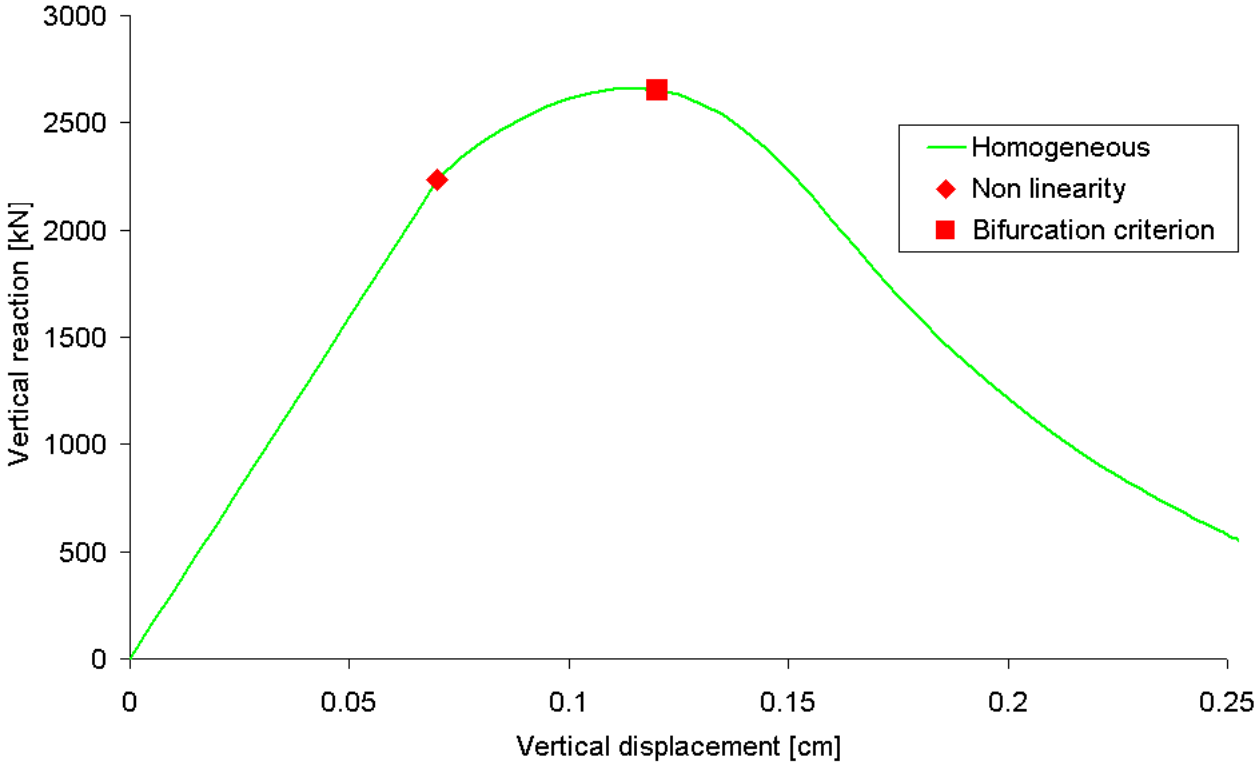
$$m = \frac{2\sin\phi}{3-\sin\phi} \qquad c = c_0 f(\gamma^p)$$

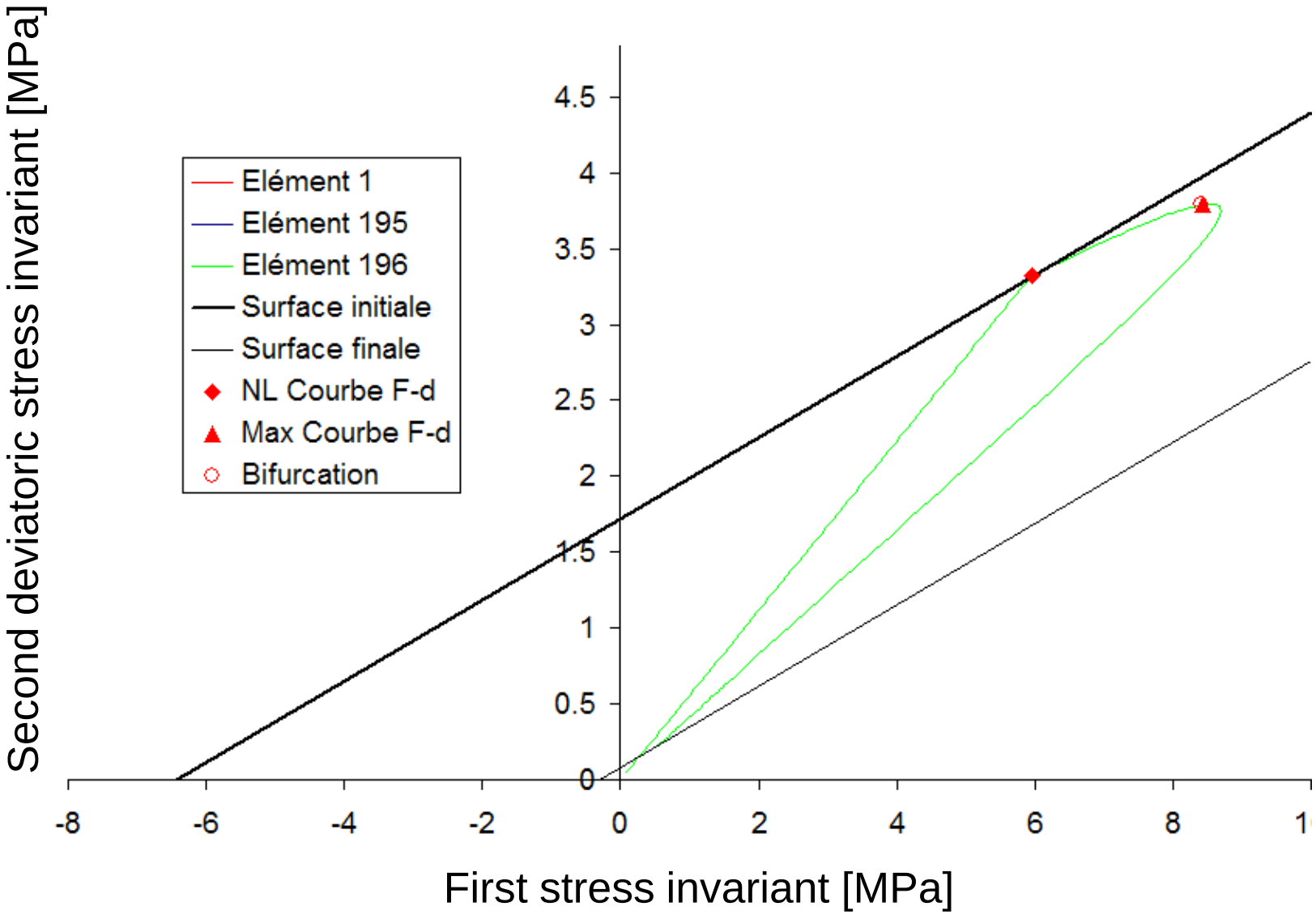
Associated softening plasticity (decrease of cohesion) :

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

$$= \alpha^2 \; si \; \gamma^p \geq \gamma_R^p$$

Softening behaviour : localization effects are very important



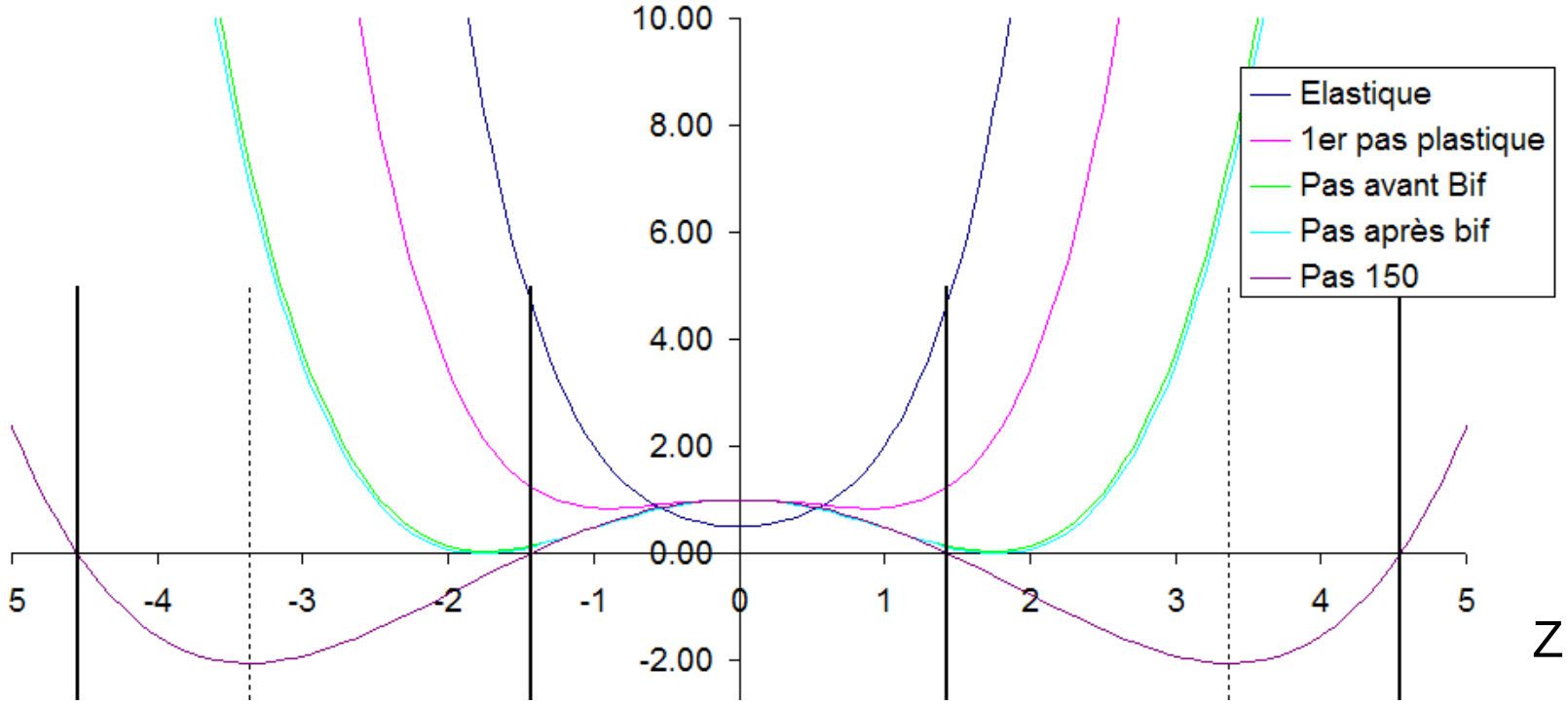

Second deviatoric stress invariant [MPa]
First stress invariant [MPa]
Elément 1
Elément 195
Elément 196
Surface initiale
Surface finale
NL Courbe F-d
Max Courbe F-d
Bifurcation
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
-8
-6
-4
-2
0
2
4
6
8
1

Softening behaviour : localization effects are very important

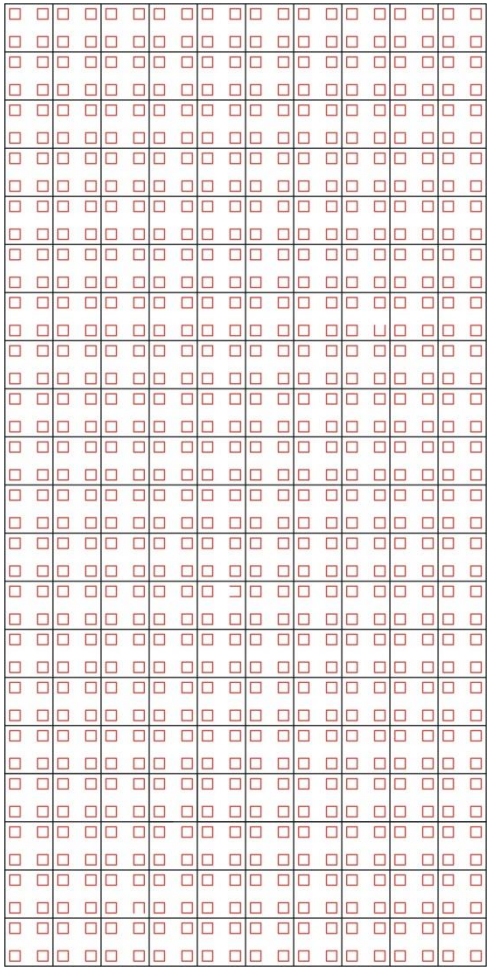
Bifurcation analysis thanks to the Rice criterion (Acoustic tensor)

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

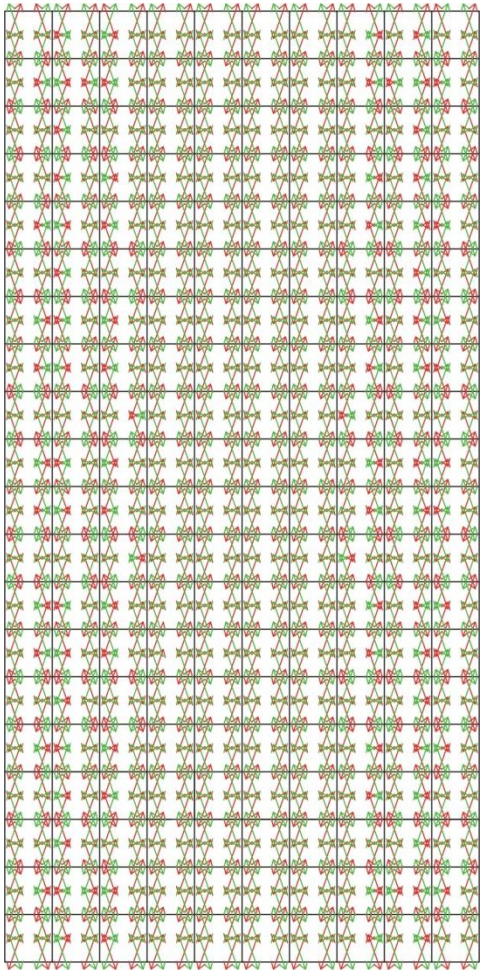
Acoustic tensor determinent



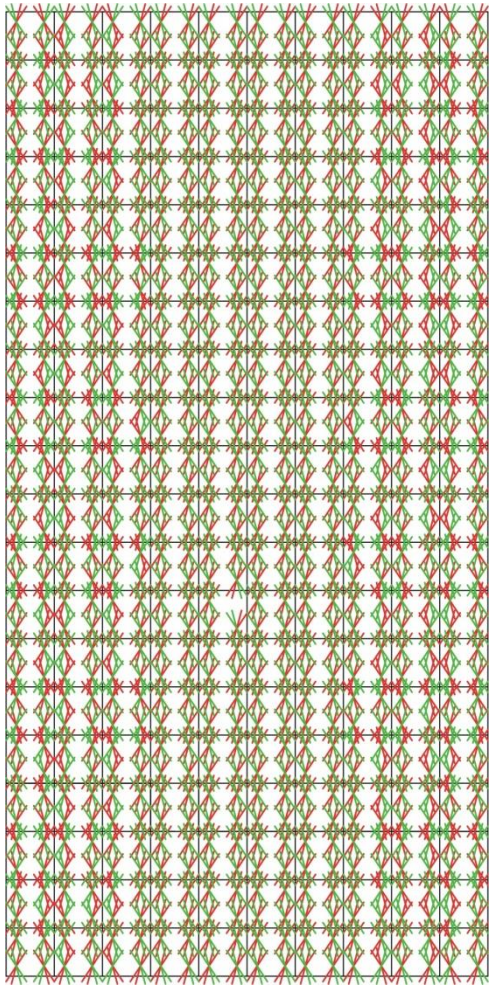
Plastic point



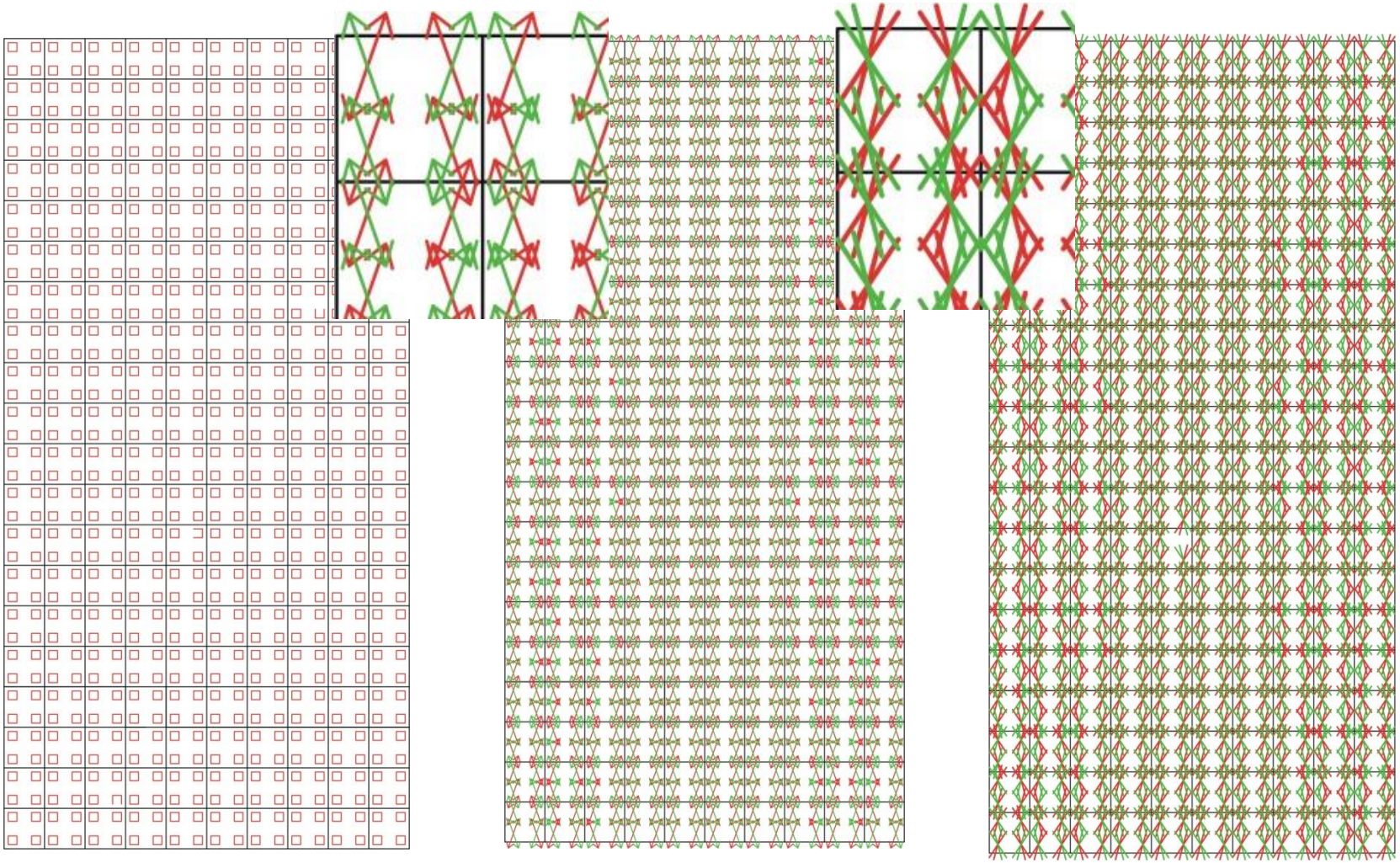
Bifurcation dir.



Bifurcation cones

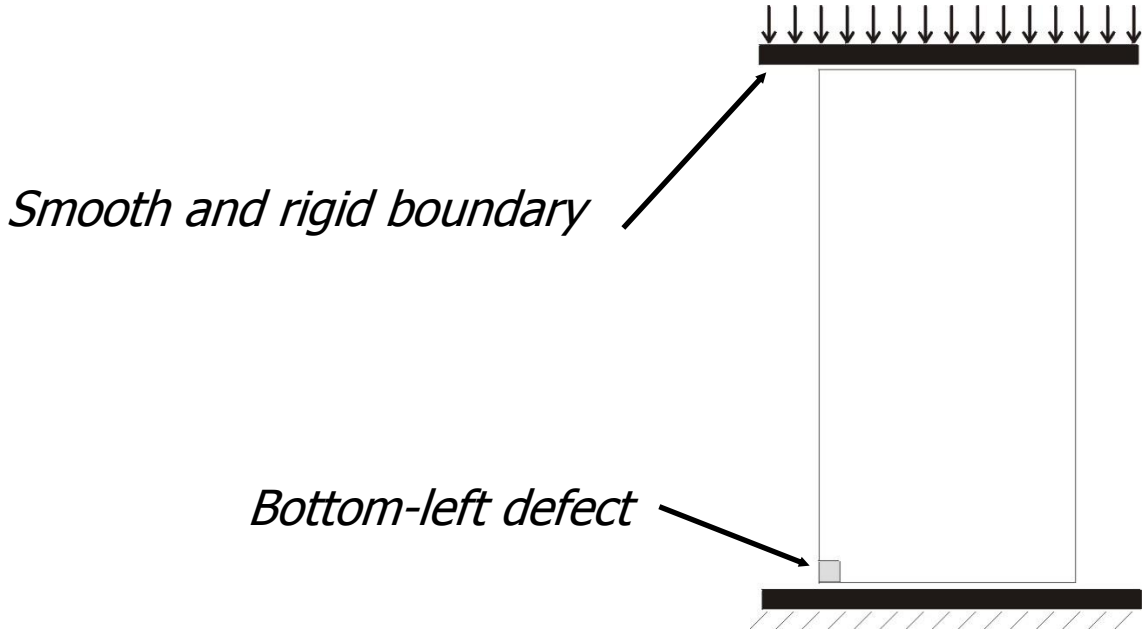


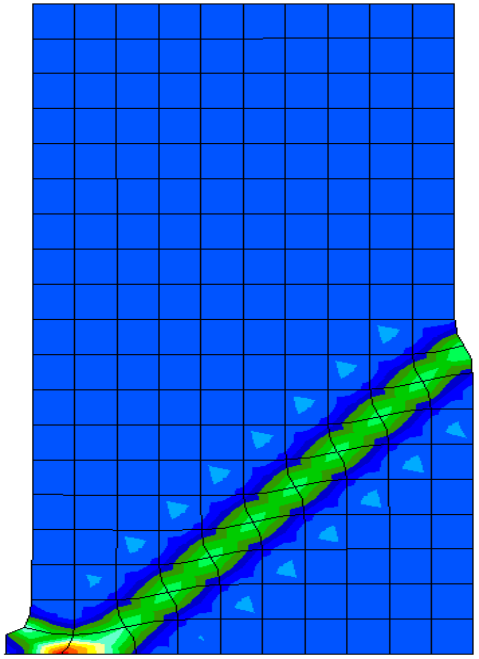
Plastic point *Bifurcation dir.* *Bifurcation cones*

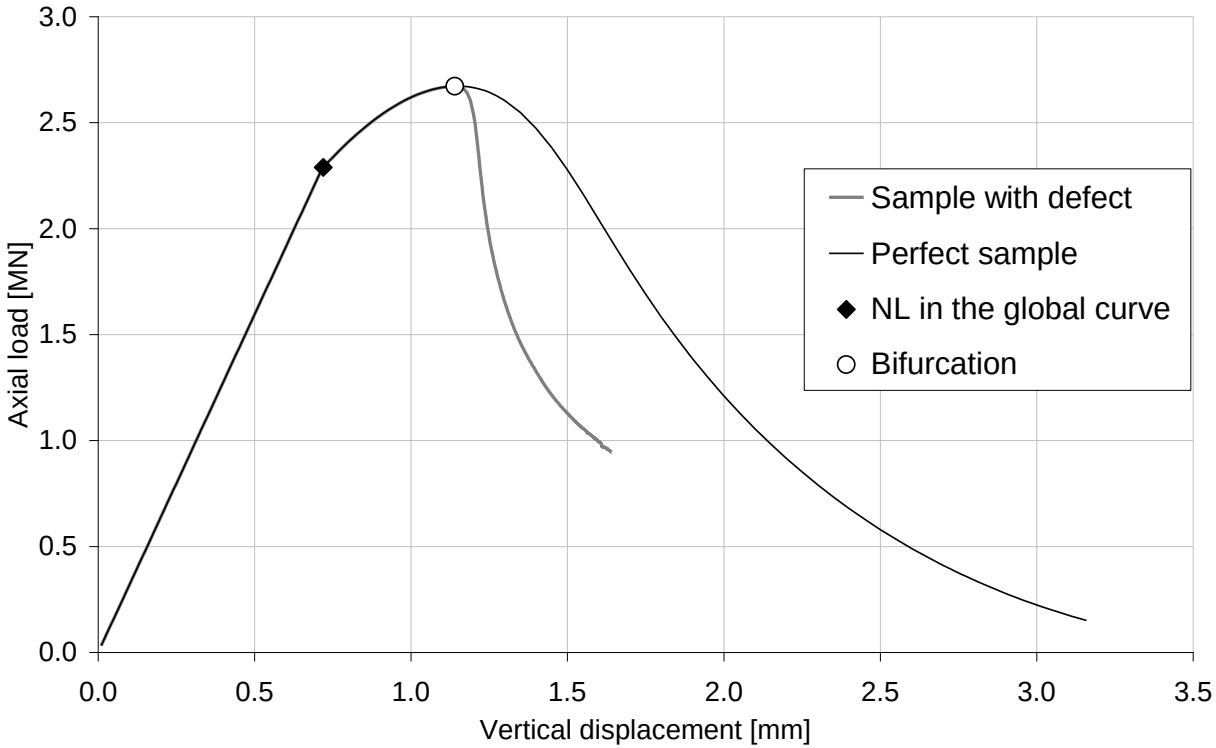


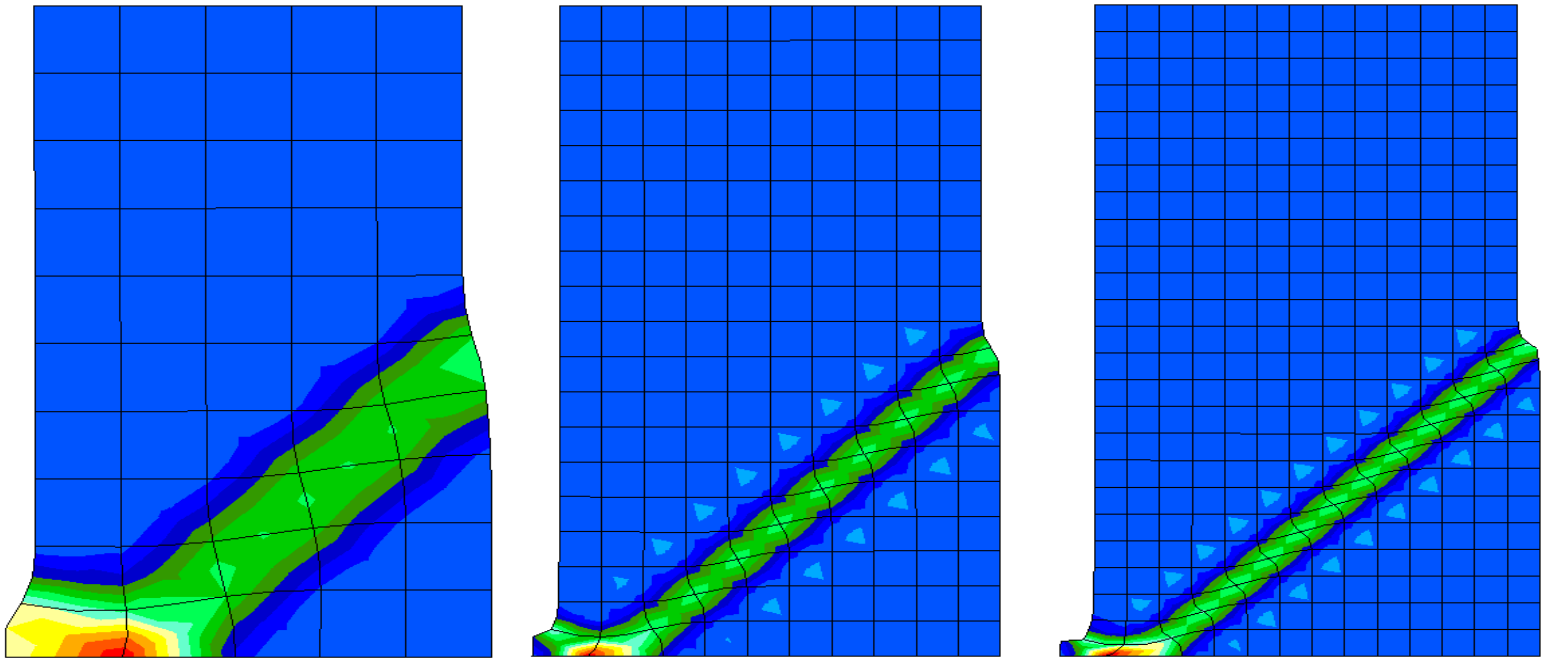
The Rice criterion provides us the information on when and how localization may appear.
Do we have any problem to model such phenomenon with classical finite element method ?

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






3.0
2.5
2.0
1.5
1.0
0.5
0.0
Axial load [MN]
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Vertical displacement [mm]
Sample with defect
Perfect sample
NL in the global curve
Bifurcation



50 elements 200 elements 300 elements

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*

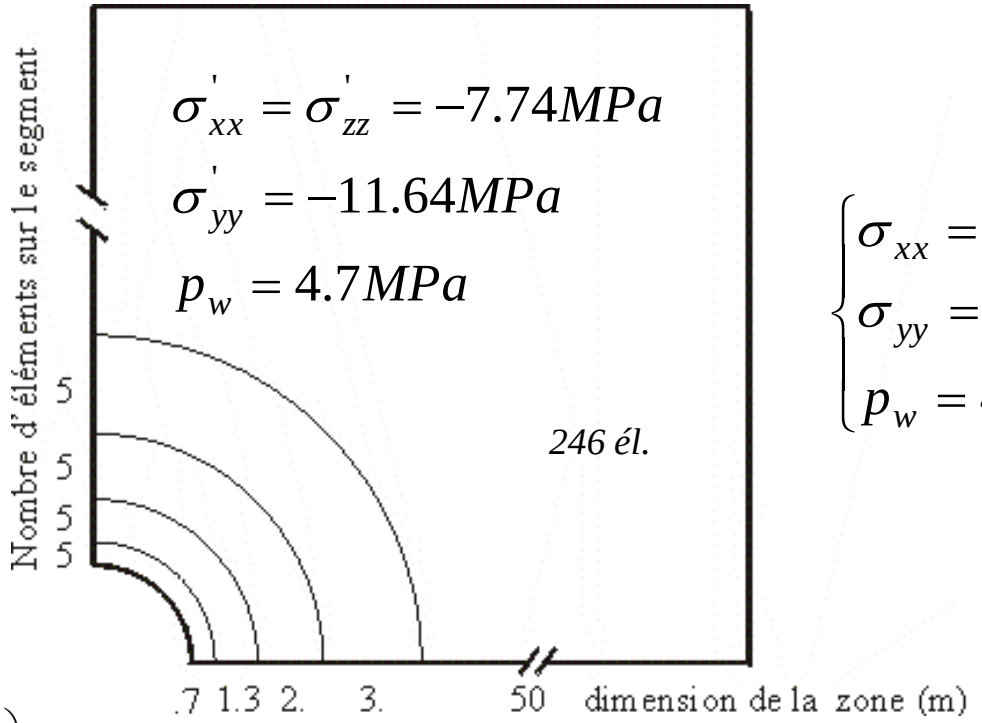
Mesh length 60 m

Choice :

Symmetry of the problem is assumed

894 elements – 2647 nodes – 7941 dof

Example of EDZ around a cavity



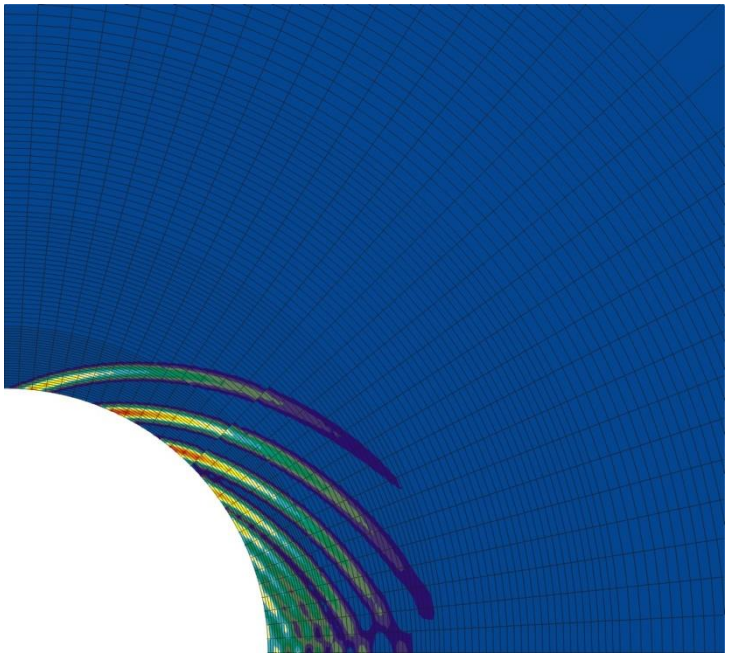
$$\begin{cases} \sigma_{xx} = -11.5MPa \\ \sigma_{yy} = -15.4MPa \\ p_w = 4.7MPa \end{cases}$$

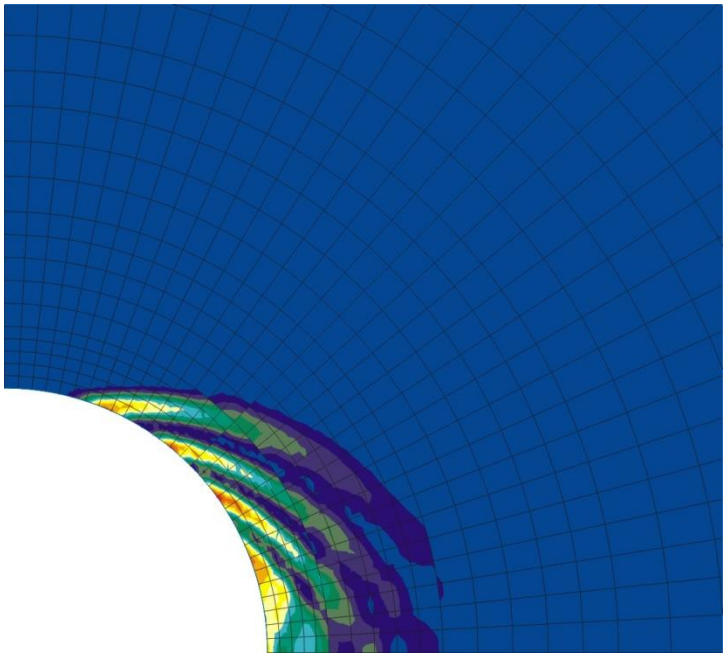
$$\begin{cases} 0 \le t \le T \\ \sigma_{xx} = \sigma'_{xx} - bS_{rw}p_w = -11.5\left(1 - \frac{t}{T}\right)MPa \\ \sigma_{yy} = \sigma'_{yy} - bS_{rw}p_w = -15.4\left(1 - \frac{t}{T}\right)MPa \\ p_w = 4.7\left(1 - \frac{t}{T}\right)MPa \\ t > T \\ \sigma_{xx} = \sigma_{yy} = p_w = 0 \end{cases}$$

T = 1.5 Ms (17 days)

t_{total} = 300 Ms (9.5 years)

Coupled modelling – Comparison Coarse mesh / Refined mesh





Deviatoric strains

Output

- Localization study : Acoustic tensor determinent
- 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*
- *Theoretical tools*
- *Numerical models*
- *Numerical application*
- *Conclusions*

- Classical FE formulation: mesh dependency
- Different regularization methods

Gradient plasticity

Enrichment of the law

Non-local approach

Microstructure continuum

Cosserat model

Enrichment of the kinematics

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:

$$R_{ij} = \frac{1}{2}(F_{ij} - F_{ji})$$

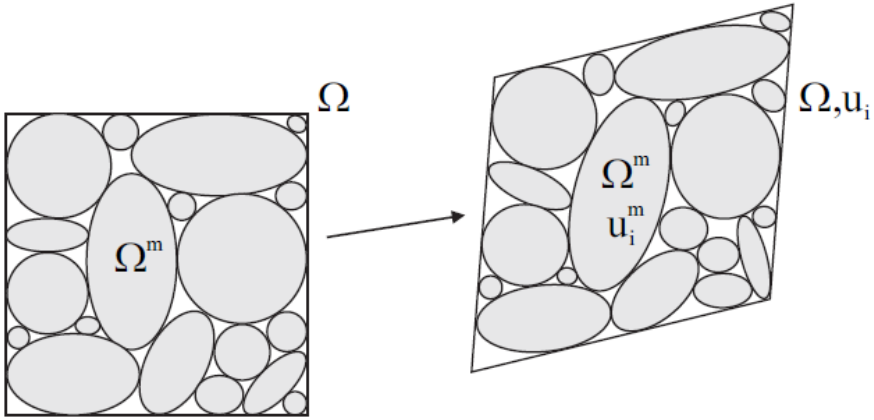
Enrichment of the kinematics :

The continuum is enriched with microstructure effects.

Macro-kinematics + micro-kinematics

Macro Ω:

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



Micro Ω^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)

$$W^{*\mathrm{i}} = \int_{\Omega} w^* \,\mathrm{d}v = \int_{\Omega} (\sigma_{ij} D^*_{ij} + \tau_{ij}(f^*_{ij} - F^*_{ij}) + \chi_{ijk} h^*_{ijk}) \,\mathrm{d}v$$

- The external virtual work (simplified)

$$W^{*\mathrm{e}} = \int_{\Omega} G_i u^*_i \,\mathrm{d}v + \int_{\partial\Omega} (t_i u^*_i + T_{ij} f^*_{ij}) \,\mathrm{d}s$$

- The virtual work equations can be extended to large strain problems

- Balance equations

$$\begin{cases} \dfrac{\partial(\boxed{\sigma_{ij}} - \boxed{\tau_{ij}})}{\partial x_j} + G_i = 0 \\[2ex] \dfrac{\partial \boxed{\chi_{ijk}}}{\partial x_k} - \tau_{ij} = 0 \end{cases}$$

- Boundary conditions

$$\begin{cases} (\sigma_{ij} - \tau_{ij}) n_j = t_i \\[2ex] \chi_{ijk} n_k = T_{ij} \end{cases}$$

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

$$\int_\Omega \left(\sigma_{ij} D^*_{ij} + \chi_{ijk} \frac{\partial^2 u^*_i}{\partial x_j \partial x_k} \right) \mathrm{d}v = \int_\Omega G_i u^*_i \, \mathrm{d}v + \int_{\partial\Omega} (p_i u^*_i + P_i D u^*_i) \, \mathrm{d}s$$

- 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

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

$$\chi_{ijk} n_j n_k = P_i$$

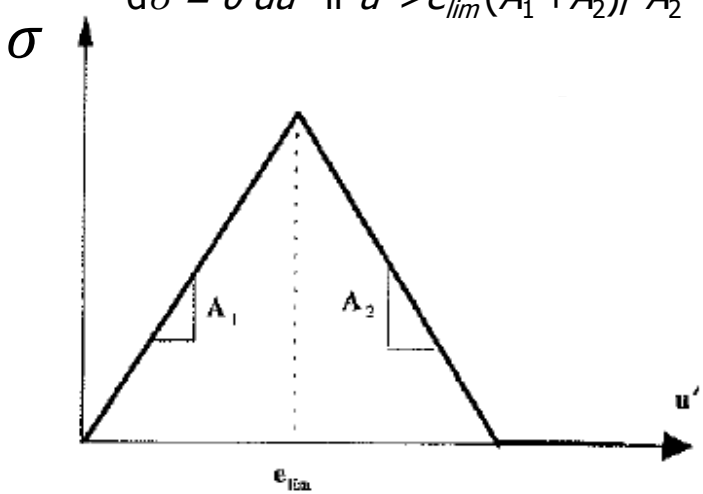
How do we introduce an internal length scale in second grade model ?

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

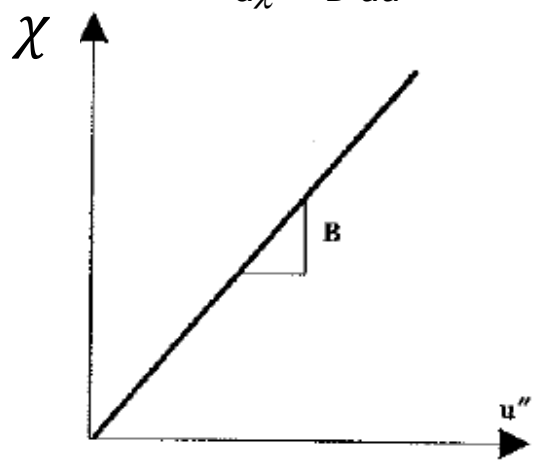
$d\sigma = A_1\, du'$ if $u' < e_{lim}$

$d\sigma = A_2\, du'$ if $u' > e_{lim}$

$d\sigma = 0\, du'$ if $u' > e_{lim}(A_1 + A_2)/A_2$



$d\chi = B\, du''$



General differential equation of the 1D problem

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

After two integrations, we obtain:

$$A.u - Bu'' = N_1 x + AK$$

Where $N_1 = \sigma - \chi' =$ Cst and $K =$ Cst,

$A = A_1$ if $u' < e_{lim}$

$A = A_2$ if $u' > e_{lim}$

General differential equation of the problem $A.u - Bu'' = N_1 x + AK$

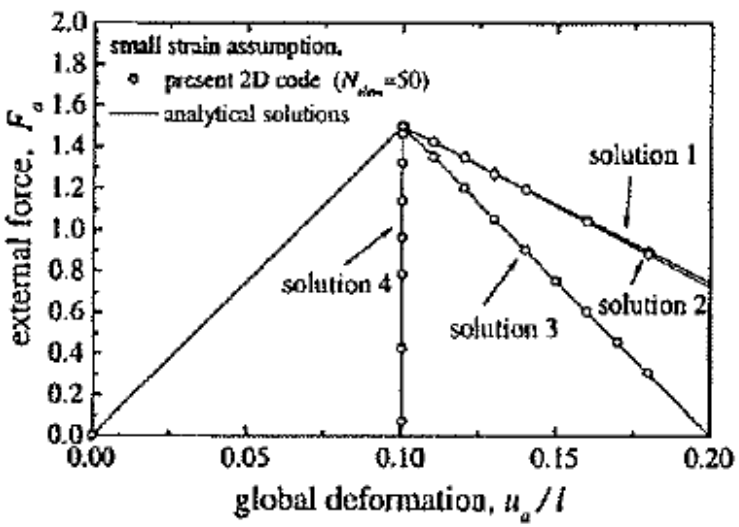
General solution of the problem

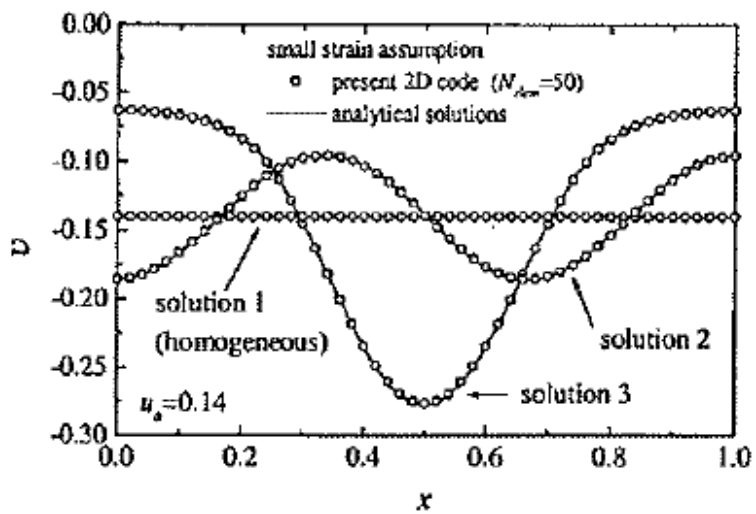
$$u = (N_1/A_1)x + K + \alpha \cosh(\omega x) + \beta \sinh(\omega x)\,; \qquad \omega^2 = A_1/B > 0$$

if $u' < e_{lim}$

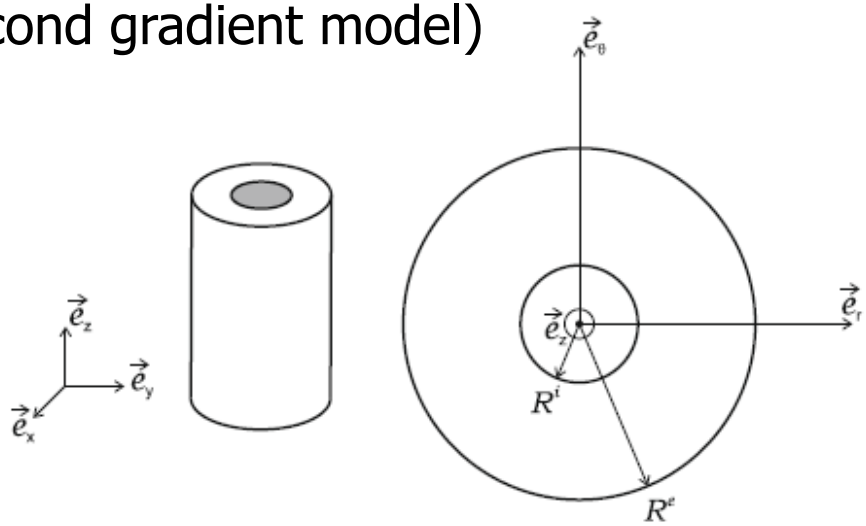
$$u = (N_1/A_1)x + K + \alpha \cos(\eta x) + \beta \sin(\eta x)\,; \qquad -\eta^2 = A_2/B < 0$$

if $u' > e_{lim}$





Let's take another example: thick-walled cylinder problem (elastic second gradient model)



Balance equation $$\partial_r(r\sigma_{rr}) - \sigma_{\theta\theta} + \frac{1}{r}\partial_r(r(\chi_{\theta\theta r} + \chi_{r\theta\theta} + \chi_{\theta r\theta})) - \partial_r^2(r\chi_{rrr}) = 0$$

General differential equation of the problem $$(\lambda + 2\mu)r\partial_r v - Br\partial_r\left(\frac{1}{r}\partial_r(r\partial_r v)\right) = 0$$

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

General solution $$u = \boxed{C_1 B^I\left(1, \frac{r}{\alpha}\right) + C_2 B^K\left(1, \frac{r}{\alpha}\right)} + \boxed{C_3 r + \frac{C_4}{r}}$$

$$\alpha = \sqrt{\frac{B}{\lambda + 2\mu}}$$

Finite element formulation of a second grade model

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

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

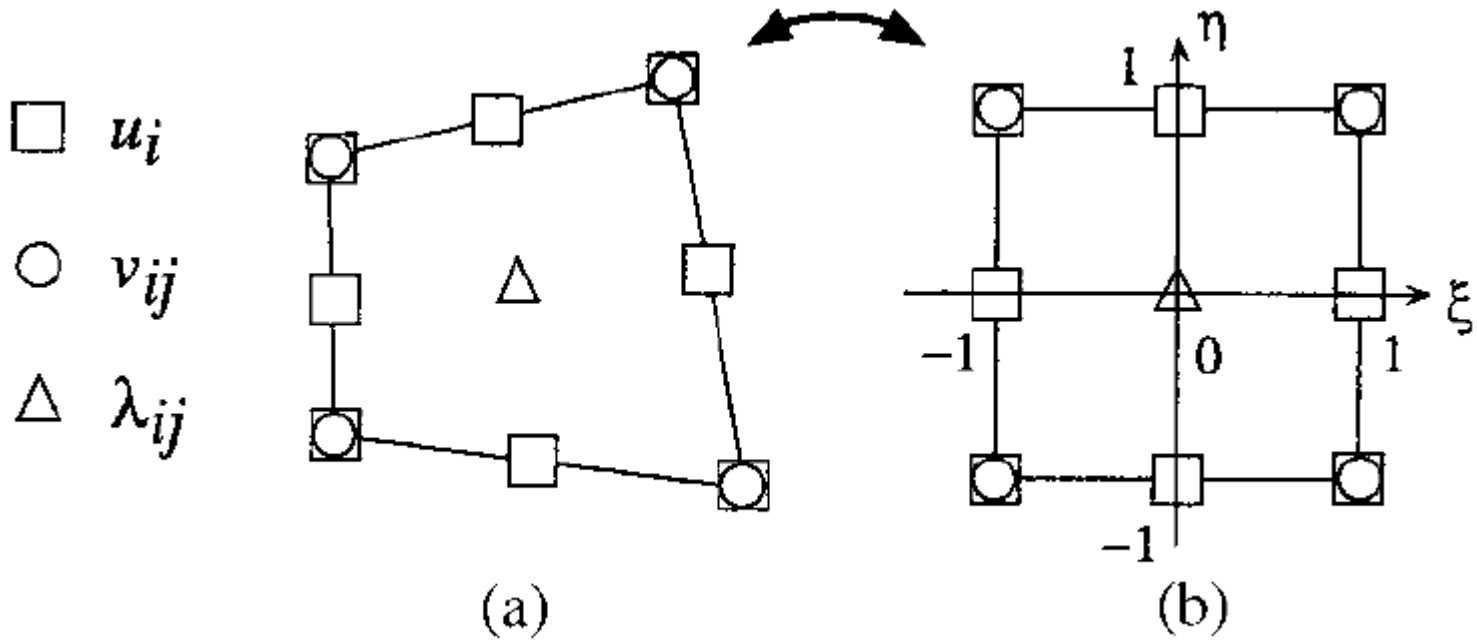
Local quantities

Introduction of Lagrange multiplier field :

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

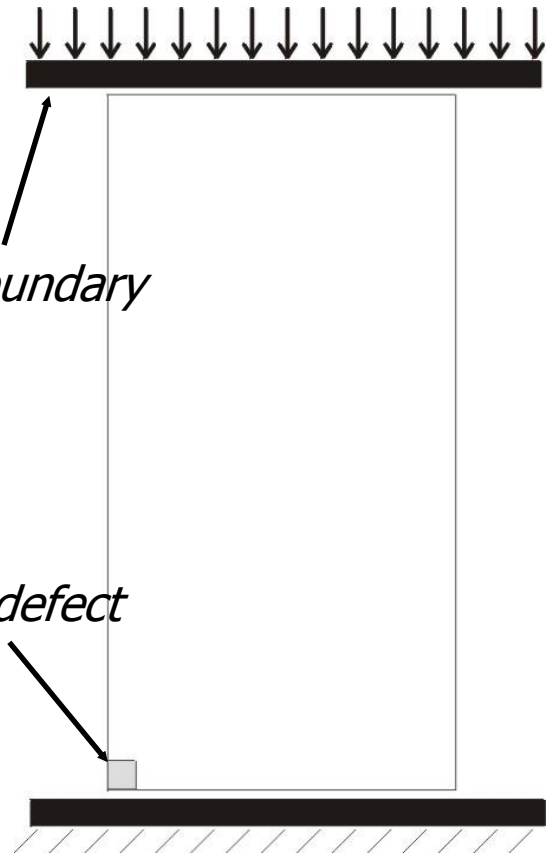
$$\int_\Omega \lambda_{ij}^* \left(\frac{\partial u_i}{\partial x_j} - v_{ij} \right) d\Omega = 0$$

Local Second gradient Finite element



Example n°1 (again)

- *Biaxial compression test*



Strain rate : 0.18% / hour

No lateral confinement

Globally drained (upper and lower drainage)

- *First gradient law :*

Linear elasticity : E_0 *and* ν_0

Drucker Prager criterion :

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

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

Associated softening plasticity (decrease of cohesion) :

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

$$= \alpha^2 \; si\; \gamma^p \geq \gamma_R^p$$

E = 5800 MPa	ϕ = 25°	c_0 = 1 MPa
ν = 0,3	Ψ = 25°	α = 0,01
		γ_R = 0,015

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

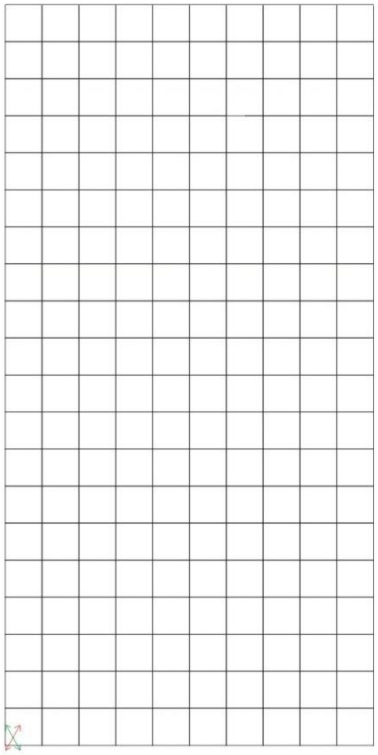
$$\begin{bmatrix} \tilde{\Sigma}_{111} \\ \tilde{\Sigma}_{112} \\ \tilde{\Sigma}_{121} \\ \tilde{\Sigma}_{122} \\ \tilde{\Sigma}_{211} \\ \tilde{\Sigma}_{212} \\ \tilde{\Sigma}_{221} \\ \tilde{\Sigma}_{222} \end{bmatrix} = \begin{bmatrix} D & 0 & 0 & 0 & 0 & \frac{D}{2} & \frac{D}{2} & 0 \\ 0 & \frac{D}{2}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

D = 20 kN

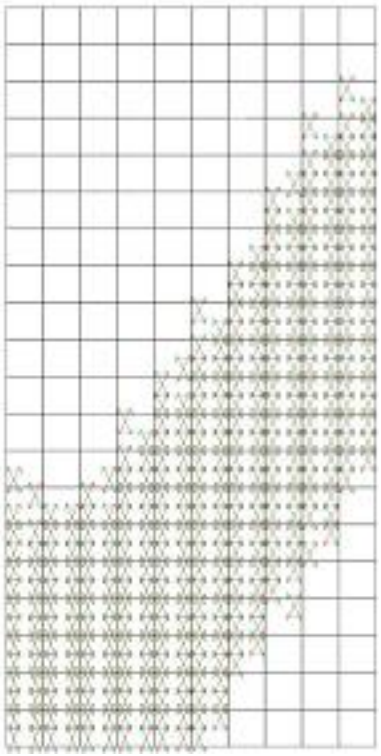
First modelling: no HM coupling (no overpressure)

Bifurcation directions

(Regularization : Second gradient)



Before

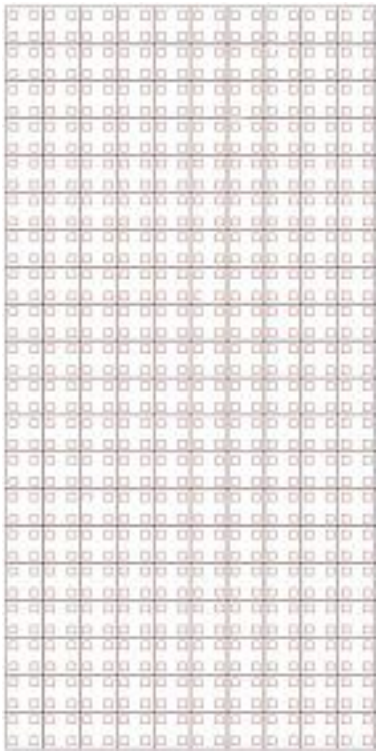


After

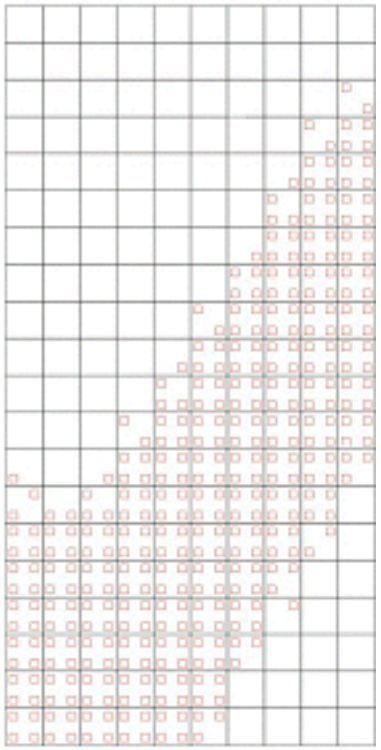
First modelling: no HM coupling (no overpressure)

Plastic loading point

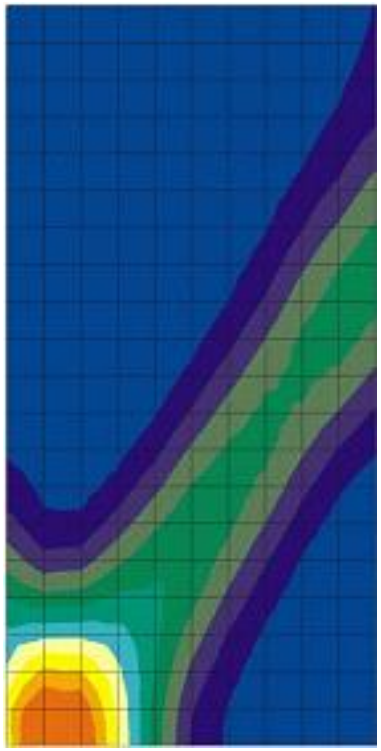
(Regularization : Second gradient)



Before



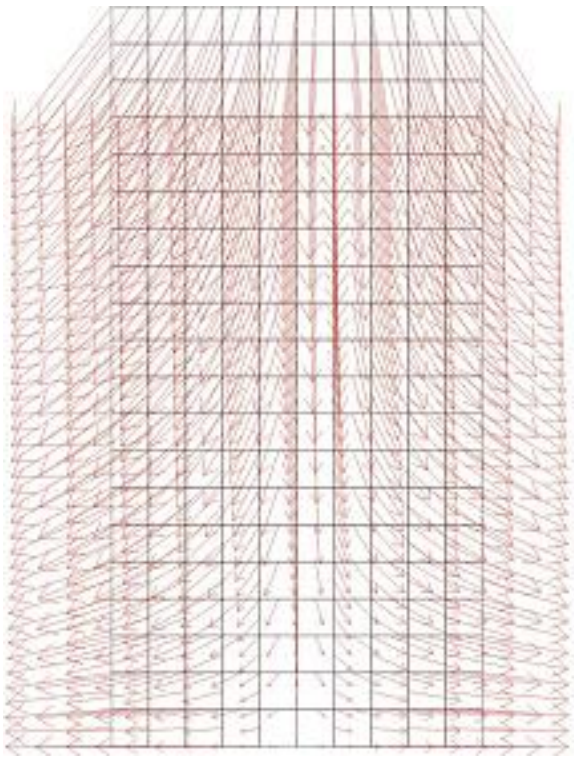
After



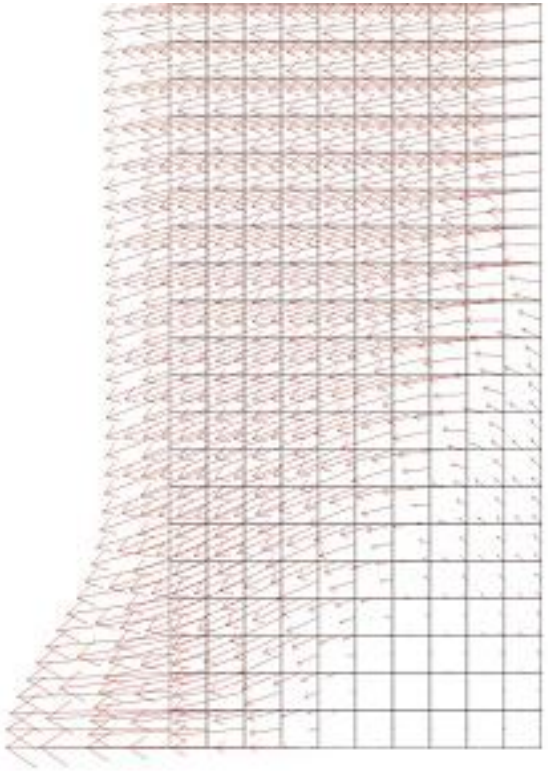
First modelling: no HM coupling (no overpressure)

Velocity field

(Regularization : Second gradient)

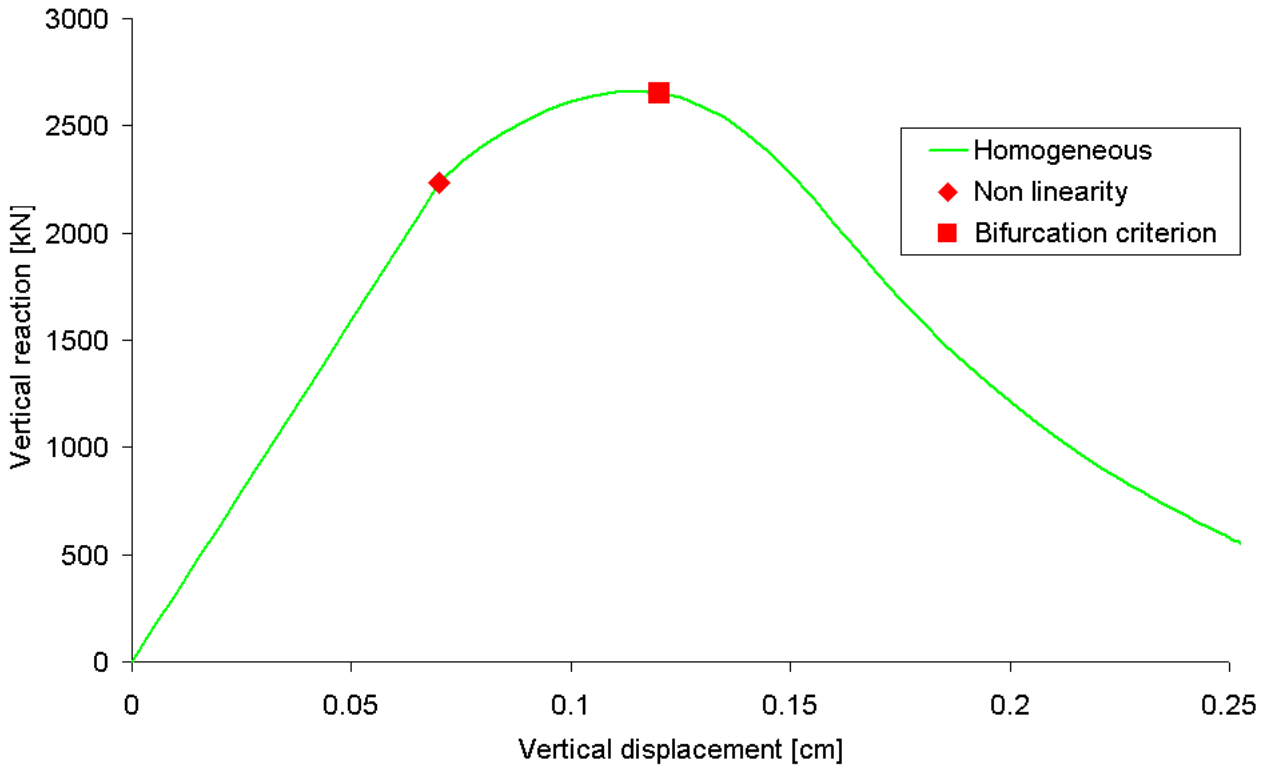


Before



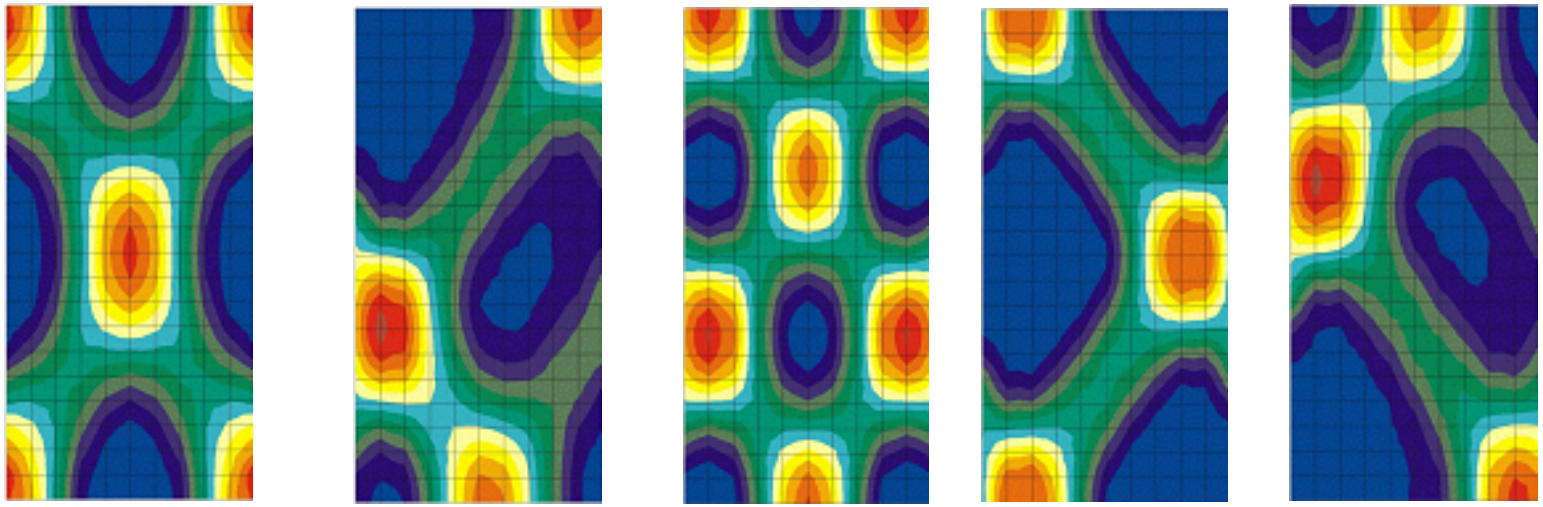
After

Initiation of localization (Directional research – Chambon et al., 2001)



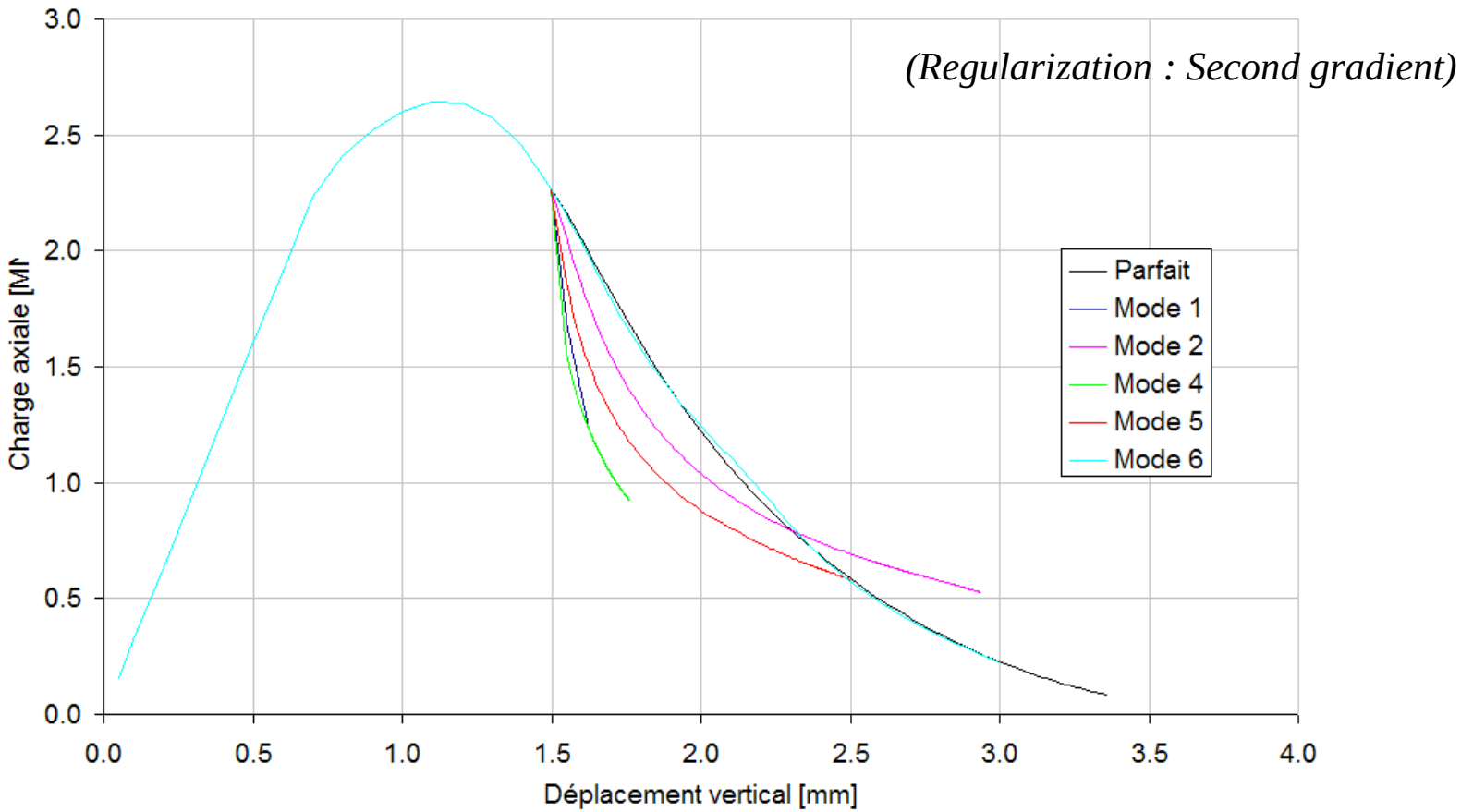
Initiation of localization (Directional research)

(Regularization : Second gradient)



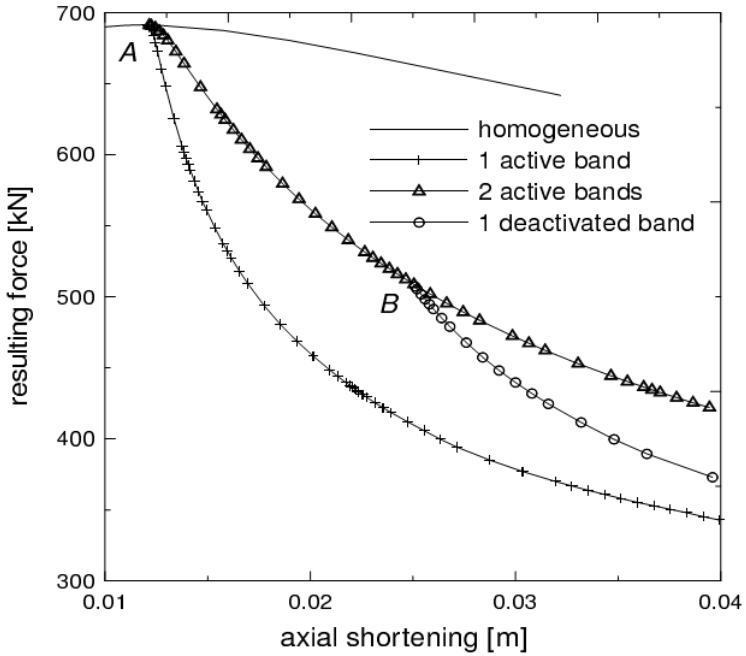
Non uniqueness of the solution

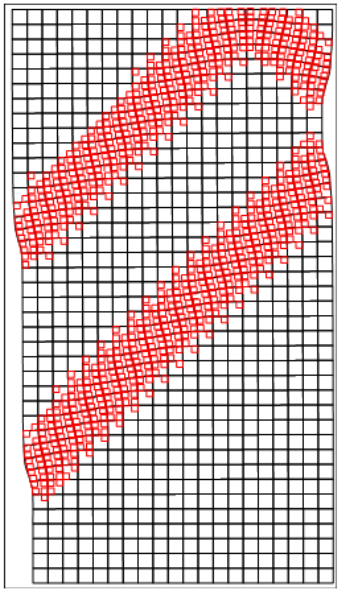
Initiation of localization (Directional research)

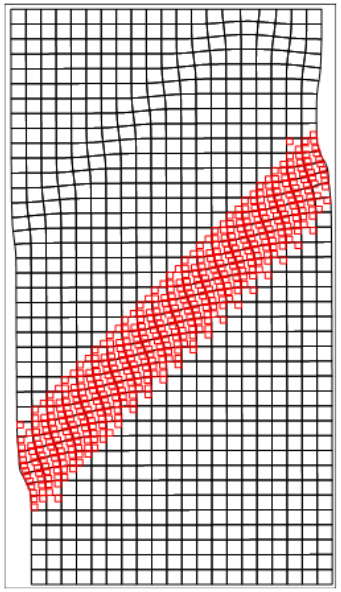


Non uniqueness of the solution

Localization mode switching (Bésuelle et al.,2006)



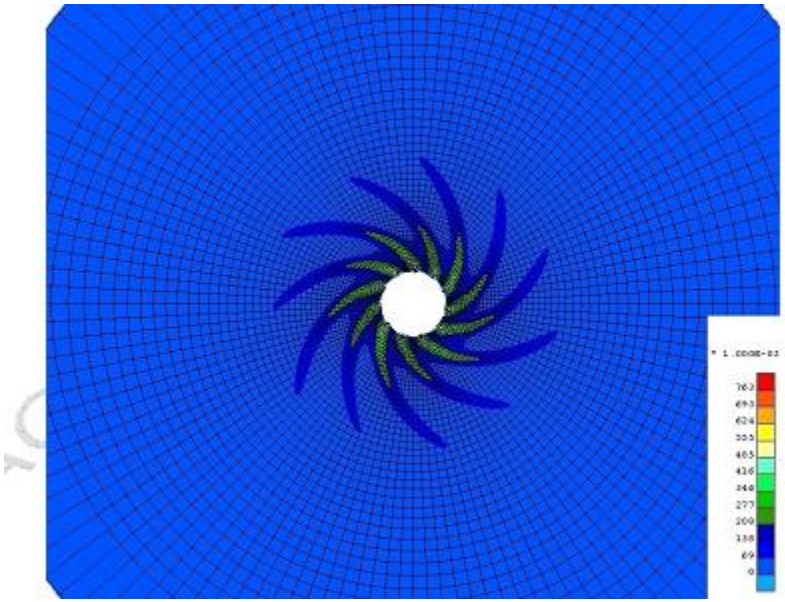


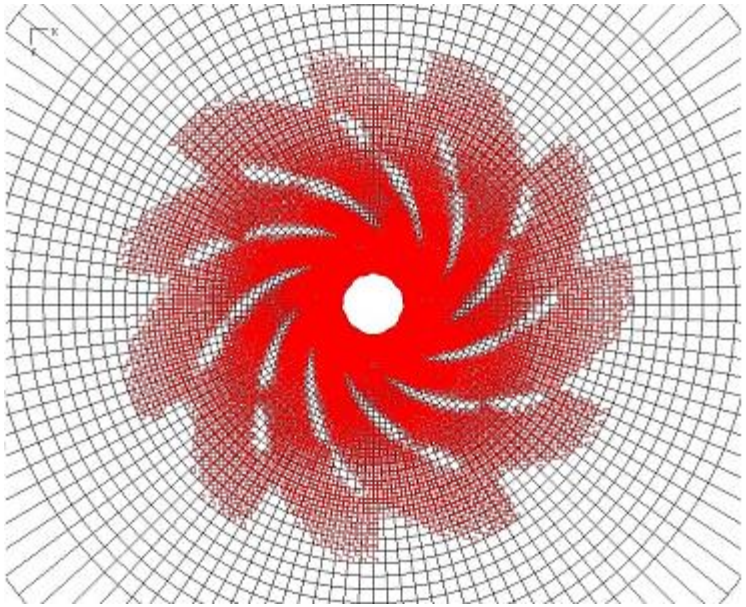


Non uniqueness of the solution

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

$$\int_{\Omega} \sigma_{ij} \varepsilon_{ij}^{*} d\Omega = \int_{\Omega} \rho_{mix} g_i u_i^{*} d\Omega + \int_{\Gamma} \bar{t}_i u_i^{*} d\Gamma$$

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 $m_i = -\rho_w \frac{\kappa}{\mu} (\frac{\partial p}{\partial x_i} + \rho_w g_i)$

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

$$\frac{\partial p^t}{\partial x_i^t} + F_i^{S/W,t} + \varrho^{w,t} g_i = 0$$

Viscous drag force : $$F_i^{S/W,t} = \frac{\varrho^{w,t}\phi^t g}{K} V_i^{W/S,t}$$

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

- *Coupled local second gradient model*

$$\int_{\Omega}\left(\sigma_{ij}\frac{\partial u_i^*}{\partial x_j}+\Sigma_{ijk}\frac{\partial^2 u_i^*}{\partial x_j \partial x_k}\right)d\Omega=\int_{\Omega}\rho_{mix}g_i u_i^* d\Omega+\int_{\Gamma}\bar{t}_i u_i^* + \bar{T}_i D u_i^* d\Gamma$$

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

- *Coupled local second gradient model*

$$\int_{\Omega}\left(\sigma_{ij}\frac{\partial u_i^*}{\partial x_j}+\Sigma_{ijk}\frac{\partial v_{ij}^*}{\partial x_k}\right)d\Omega-\int_{\Omega}\lambda_{ij}\left(\frac{\partial u_i^*}{\partial x_j}-v_{ij}^*\right)d\Omega=$$

$$\int_{\Omega}\rho_{mix}g_i u_i^* d\Omega+\int_{\Gamma}\overline{t}_i u_i^*+\overline{T}_i Du_i^* d\Gamma$$

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

$$\int_{\Omega}\lambda_{ij}^*\left(\frac{\partial u_i}{\partial x_j}-v_{ij}\right)d\Omega=0$$

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+Δt*

$$\int_{\Omega^{\tau 1}} \left(\sigma_{ij}^{\tau 1} \frac{\partial u_i^*}{\partial x_j^{\tau 1}} + \Sigma_{ijk}^{\tau 1} \frac{\partial v_{ij}^*}{\partial x_k^{\tau 1}} \right) d\Omega^{\tau 1} - \int_{\Omega^{\tau 1}} \lambda_{ij}^{\tau 1} \left(\frac{\partial u_i^*}{\partial x_j^{\tau 1}} - v_{ij}^* \right) d\Omega^{\tau 1} -$$

$$\int_{\Omega^{\tau 1}} (\varrho^s (1 - \phi^{\tau 1}) + \varrho^{w,\tau 1} \phi^{\tau 1}) g_i u_i^* d\Omega^{\tau 1} - \int_{\Gamma^{\tau 1}} \left(\overline{t}_i u_i^* + \overline{T}_i v_{ik}^* n_k^{\tau 1} \right) d\Gamma^{\tau 1} = R^{\tau 1},$$

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

$$\int_{\Omega^{\tau 1}} (\dot{M}^{\tau 1} p^\star - m_i^{\tau 1} \frac{\partial p^\star}{\partial x_i^{\tau 1}}) d\Omega^{\tau 1} - \int_{\Omega^{\tau 1}} Q^{\tau 1} p^\star d\Omega^{\tau 1} + \int_{\Gamma_q^{\tau 1}} \overline{q}^{\tau 1} p^\star d\Gamma^{\tau 1} = W^{\tau 1}.$$

R, S and W : Residuals of the balance equations

- *Linearization of field equations*

Auxiliary linear problem

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

R, S and W : Residuals of the balance equations

$$\left[dU_{(x,y)}\right] = \left[\frac{\partial du_1}{\partial x_1} \frac{\partial du_1}{\partial x_2} \frac{\partial du_2}{\partial x_1} \frac{\partial du_2}{\partial x_2} du_1\, du_2 \frac{\partial dp}{\partial x_1} \frac{\partial dp}{\partial x_2} dp \right.$$
$$\left. \frac{\partial dv_{11}}{\partial x_1} \frac{\partial dv_{11}}{\partial x_2} \frac{\partial dv_{12}}{\partial x_1} \cdots \frac{\partial dv_{22}}{\partial x_2} dv_{11} \cdots dv_{22}\; d\lambda_{11} \cdots d\lambda_{22} \right]$$

$$[E]=\begin{bmatrix} E1_{(4x4)} & 0_{(4x2)} & K_{WM\,(4x3)} & 0_{(4x8)} & 0_{(4x4)} & -I_{(4x4)} \\ G1_{(2x4)} & 0_{(2x2)} & G2_{(2x3)} & 0_{(2x8)} & 0_{(2x4)} & 0_{(2x4)} \\ K_{MW\,(3x4)} & 0_{(3x2)} & K_{WW\,(3x3)} & 0_{(3x8)} & 0_{(3x4)} & 0_{(3x4)} \\ E2_{(8x4)} & 0_{(8x2)} & 0_{(8x3)} & D_{(8x8)} & 0_{(8x4)} & 0_{(8x4)} \\ E3_{(4x4)} & 0_{(4x2)} & 0_{(4x3)} & 0_{(4x8)} & 0_{(4x4)} & I_{(4x4)} \\ E4_{(4x4)} & 0_{(4x2)} & 0_{(4x3)} & 0_{(4x8)} & -I_{(4x4)} & 0_{(4x4)} \end{bmatrix}$$

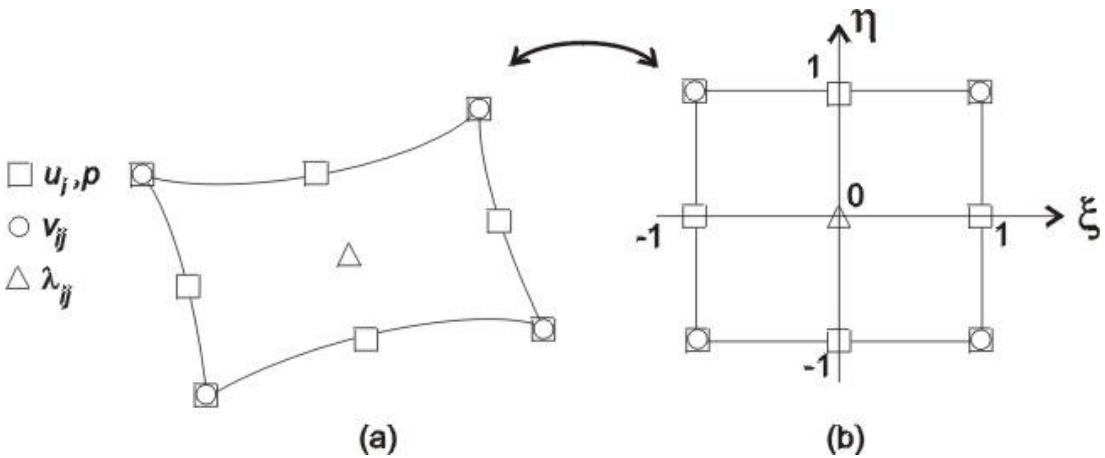
E1, E2, E3, E4 and D : see monophasic local sec. Gradient model

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*

$$\left[U^*_{node}\right]^T \int_{-1}^{1}\int_{-1}^{1} [B]^T [T]^T [E][T][B] \det J \; d\xi d\eta \left[dU_{node}\right] \equiv$$

$$\left[U^*_{node}\right]^T [k]\left[dU_{node}\right]$$

Local stiffness matrix

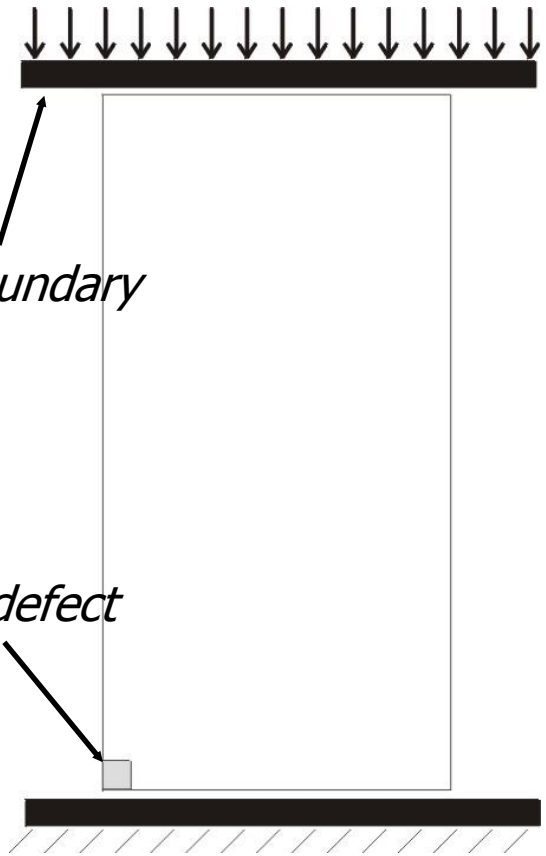
$$-R - S - W = P^*_{ext} - \left[U^*_{node}\right]^T \int_{-1}^{1}\int_{-1}^{1} [B]^T [T]^T [\sigma] \det J \; d\xi d\eta \equiv$$

$$\left[U^*_{node}\right]^T \left[f_{HE}\right]$$

Elementary out of balance forces

Example n°1 (last time)

- *Biaxial compression test*



Strain rate : 0.18% / hour

No lateral confinement

Globally drained (upper and lower drainage)

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

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

D = 20 kN

- *Flow model parameters*

$\kappa = 10^{-19} / 10^{-12}\ m^2$

$\rho_w = 1000\ kg/m^3$

$\phi = 0.15$

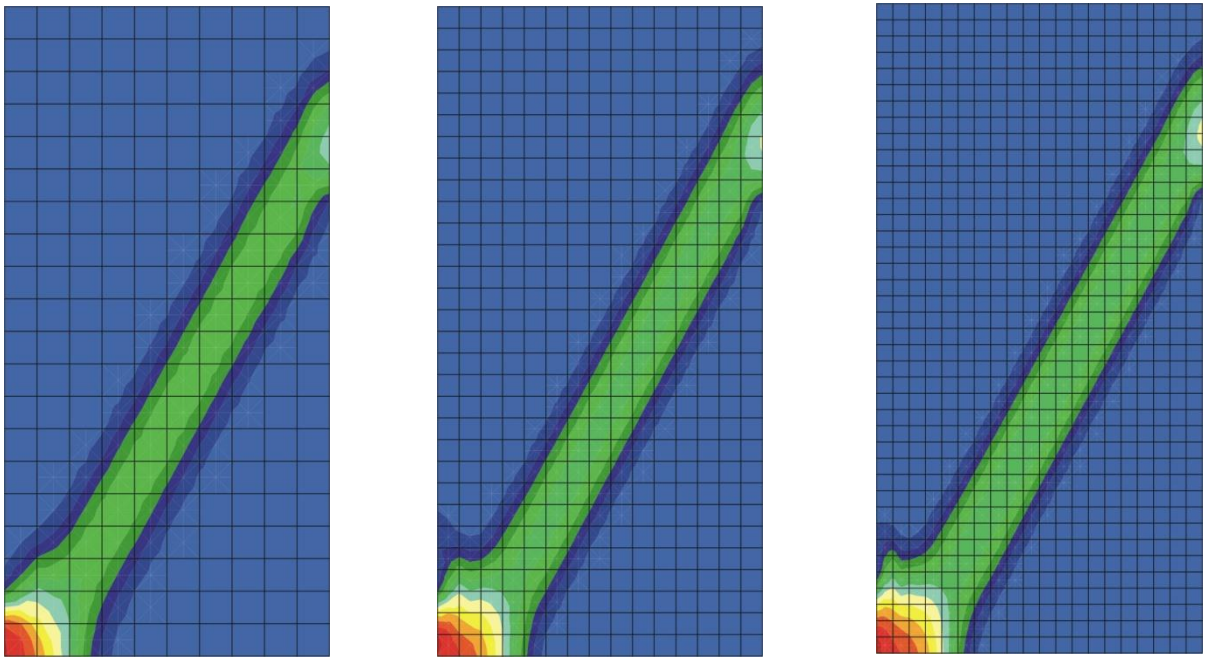
$k_w = 510^{-10}\ Pa^{-1}$

$\mu_w = 0.001\ Pa.s$

Second modelling: HM coupling

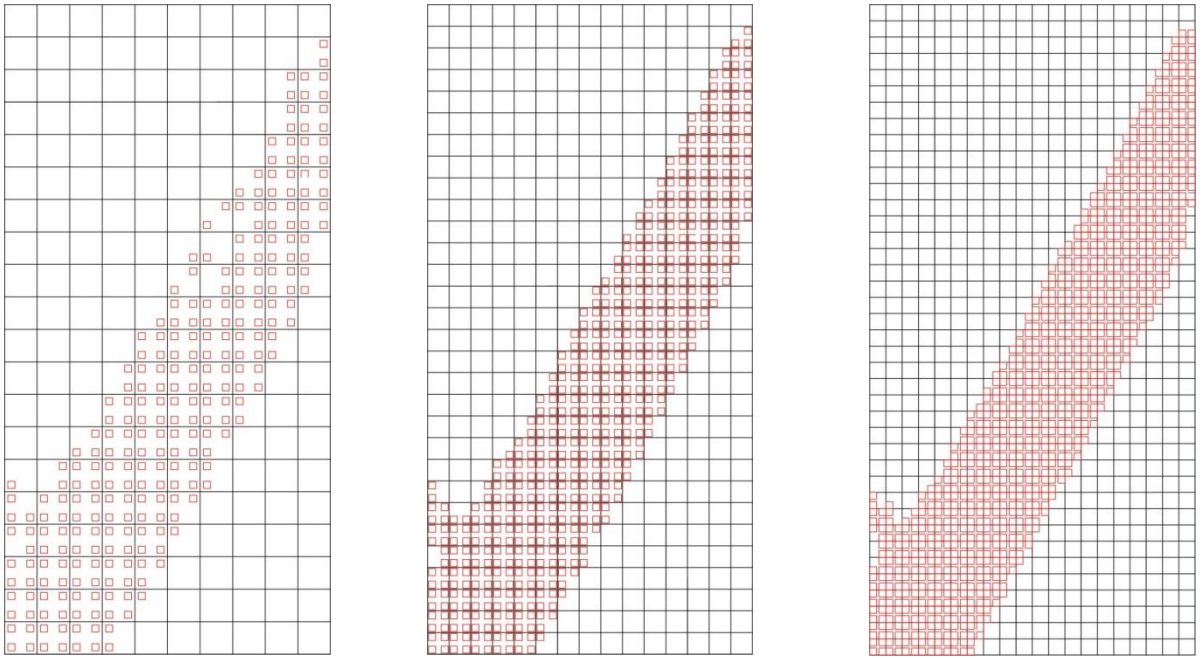
- *Equivalent strain after 0.2 % of axial strain ($\kappa = 10^{-12}$ m²)*

(20 x 10) *(30 x 15)* *(40 x 20)*

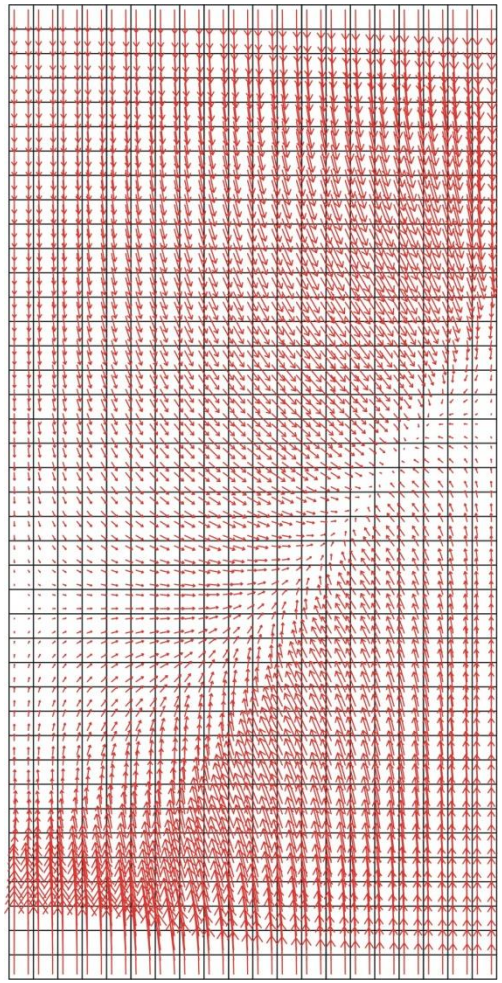


- *Plastic loading point after 0.2 % of axial strain ($\kappa = 10^{-12}$ m²)*

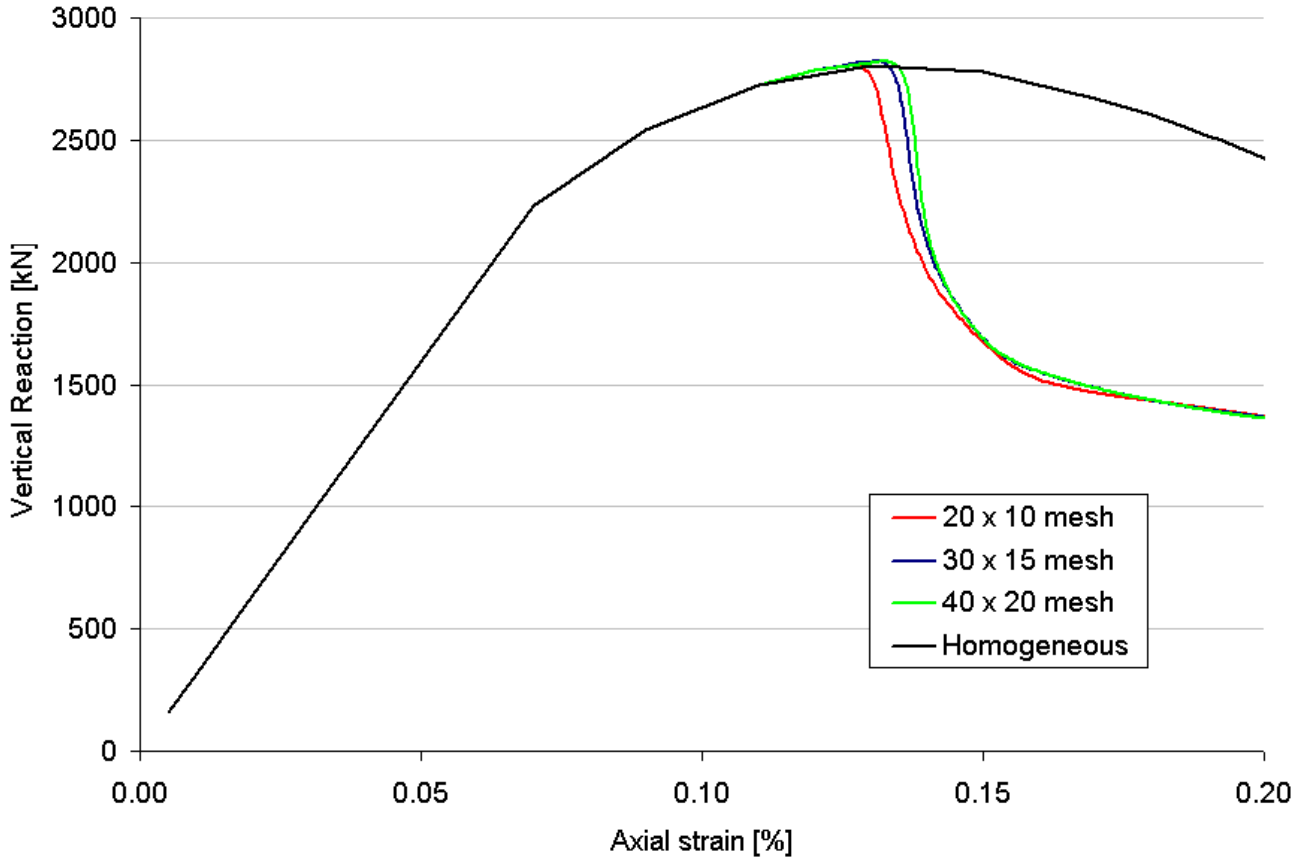
(20 x 10) *(30 x 15)* *(40 x 20)*



- *Fluid flow after 0.2 % of axial strain ($\kappa = 10^{-12}$ m²)*

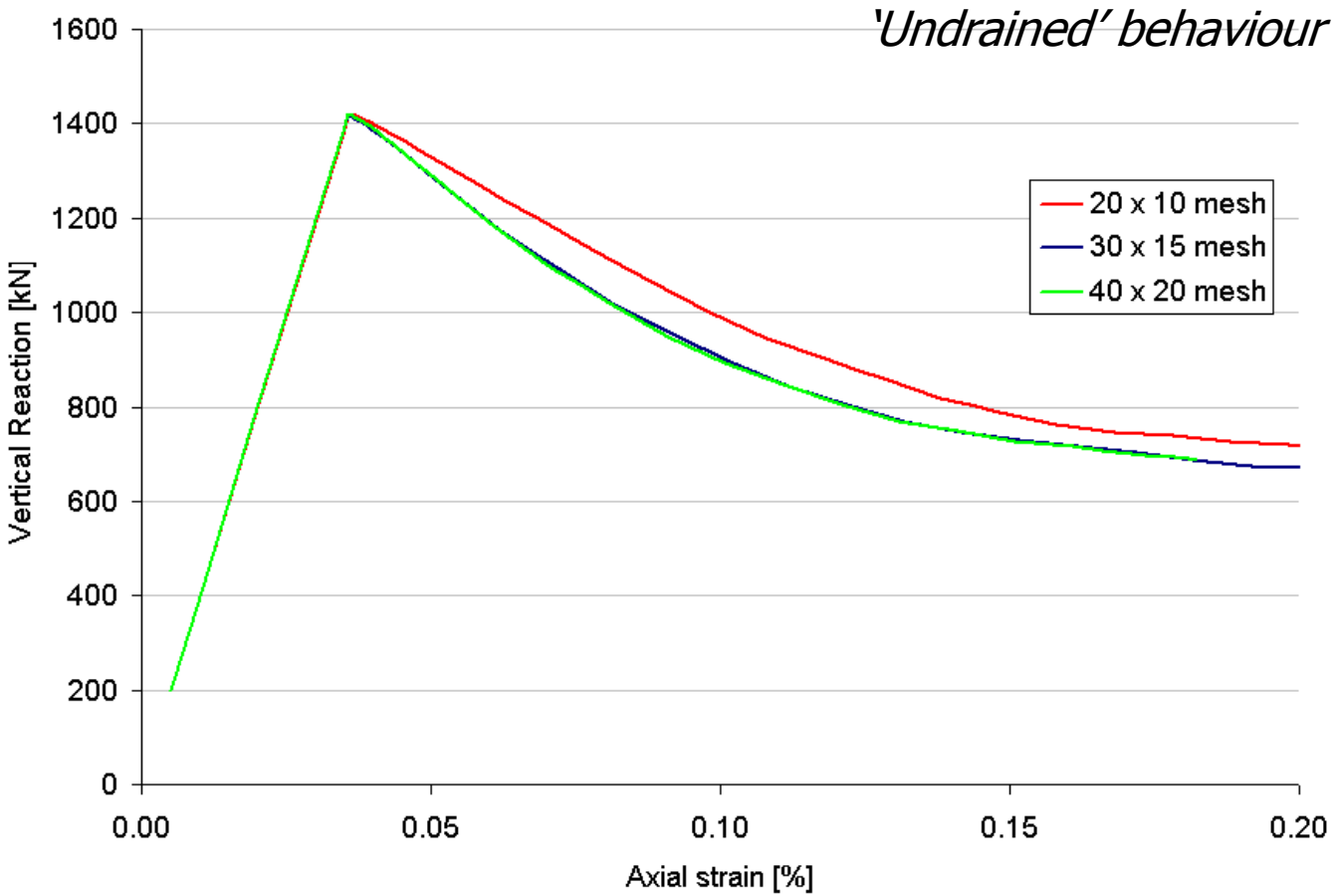


- *Load-displacement curve ($\kappa = 10^{-12}$ m²)*

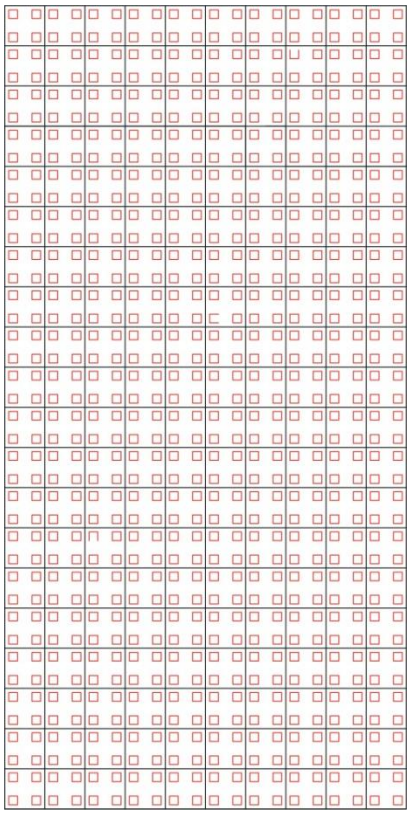


Second modelling: HM coupling

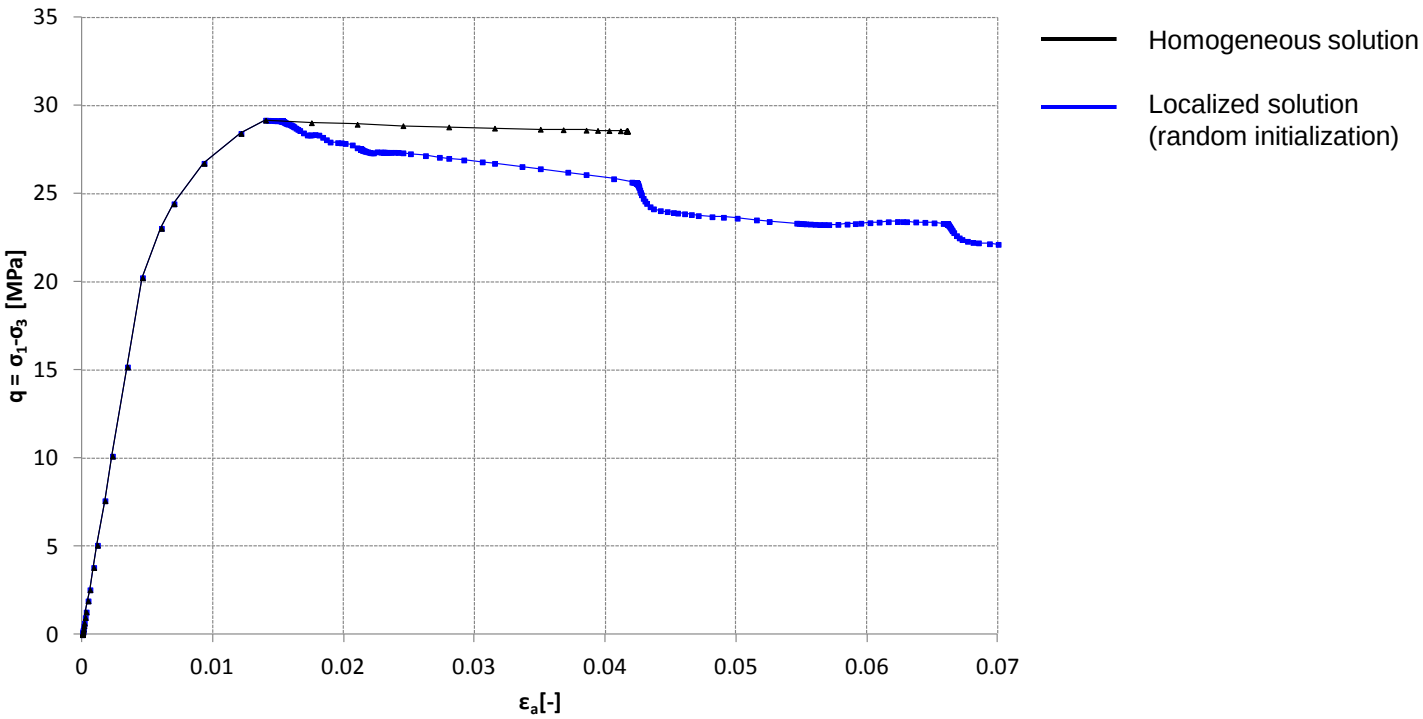
- *Load-displacement curve ($\kappa = 10^{-19}$ m²)*



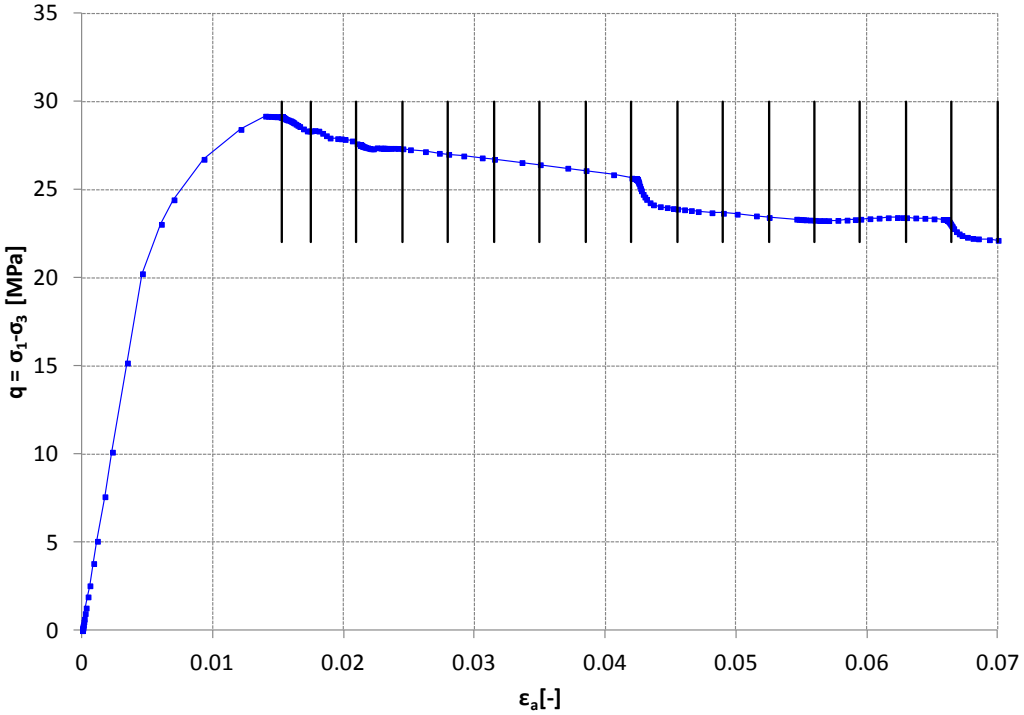
For $\kappa = 10^{-19}\ m^2$, the behaviour is undrained, we recover the experimental observation showing that for dilatant material, no localization is possible before cavitation.



Random initialization (coupled problem)



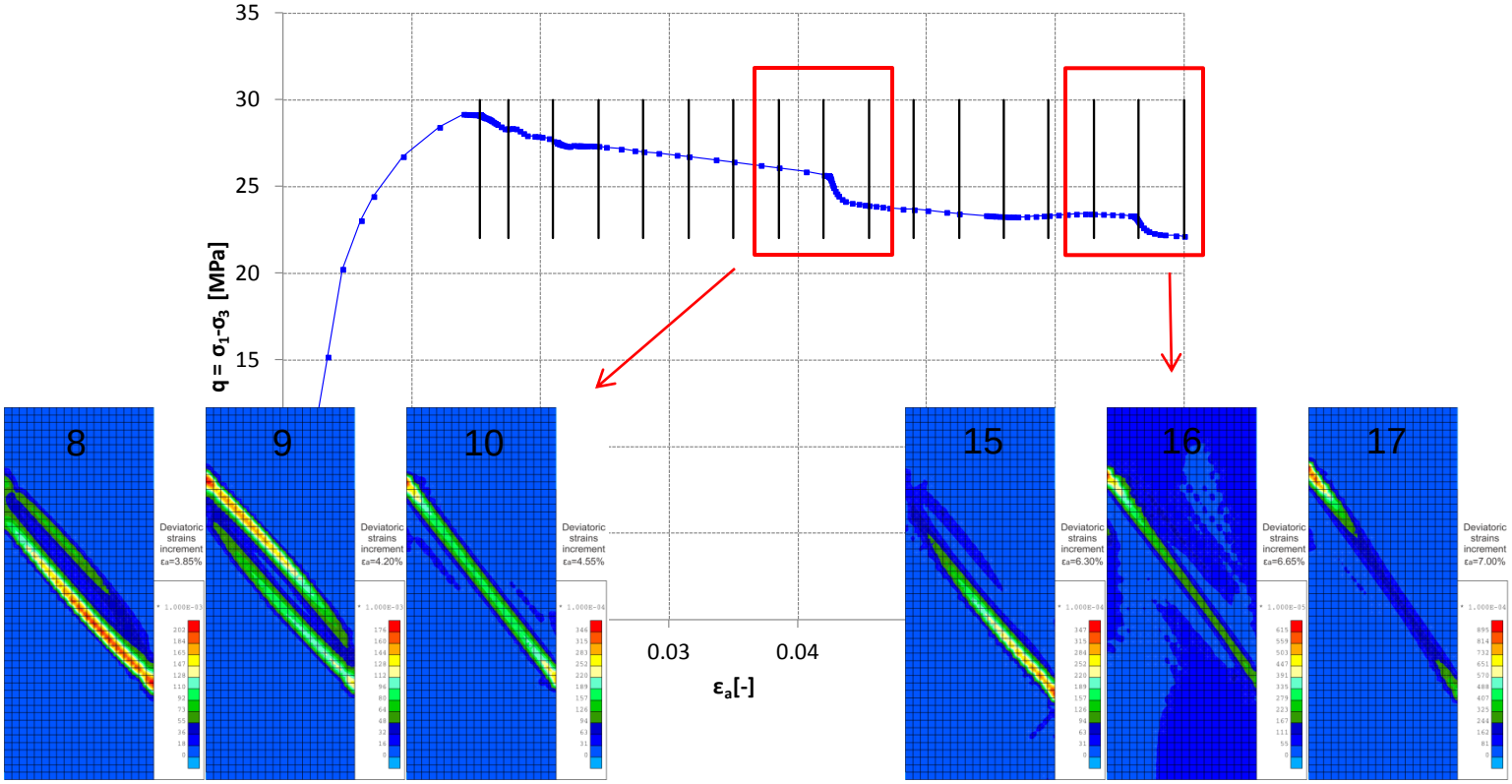
Random initialization (coupled problem)



Deviatoric strain increment

Random initialization (coupled problem)

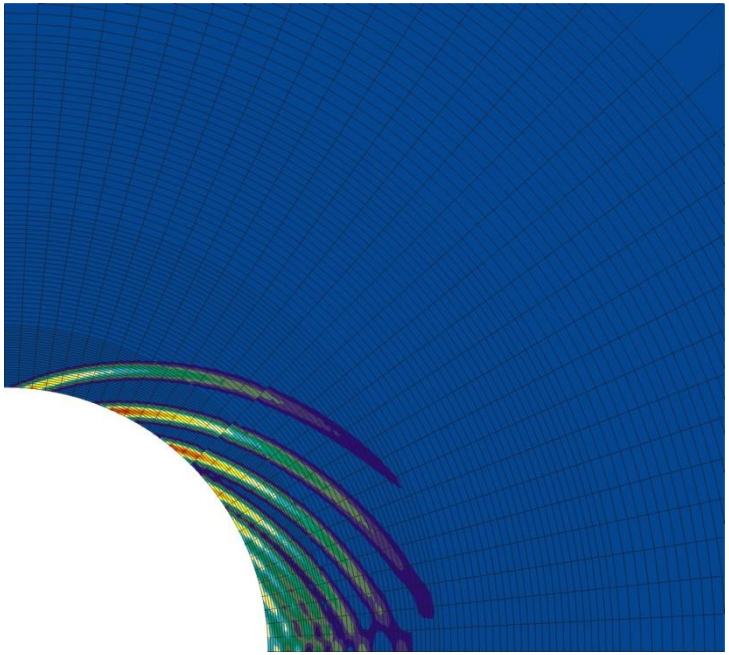
Deviatoric strain increment

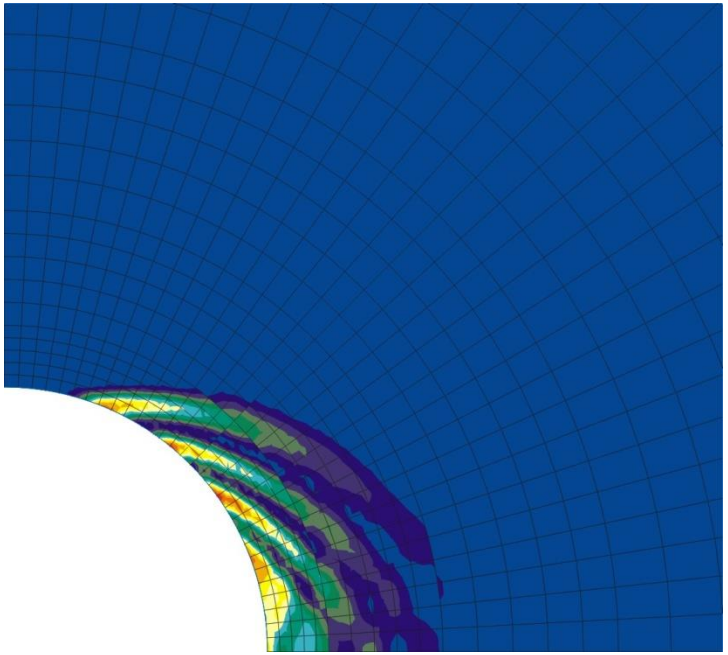


Decrease of q = disappearance of a shear band

Coupled modelling – Comparison Coarse mesh - Refined mesh

Classical FE formulation

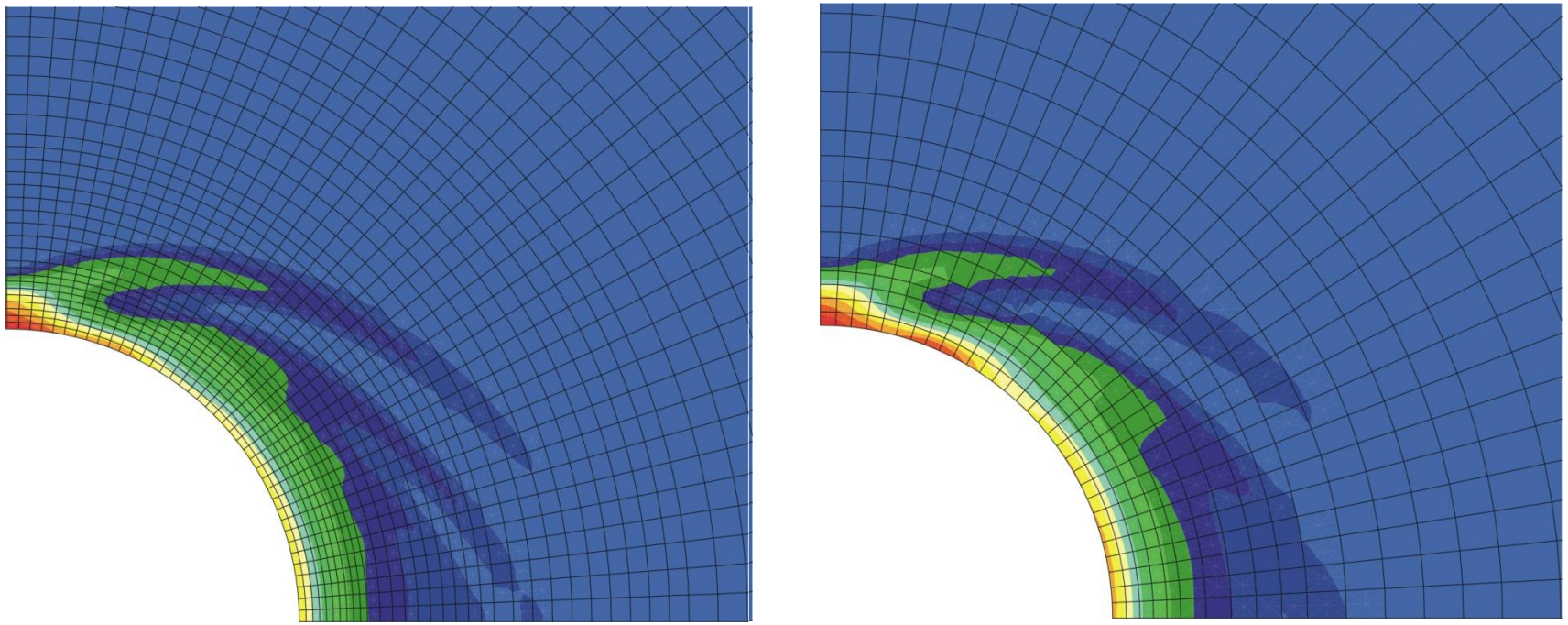




Deviatoric strains

Coupled modelling – Comparison Coarse mesh - Refined mesh

Coupled second gradient FE formulation



Deviatoric strains

Outline:

- *Introduction*
- *Theoretical tools*
- *Numerical models*
- *Numerical application*
- *Conclusions*

Long-term management of radioactive wastes

Intermediate
(long-lived)
&
high activity
wastes

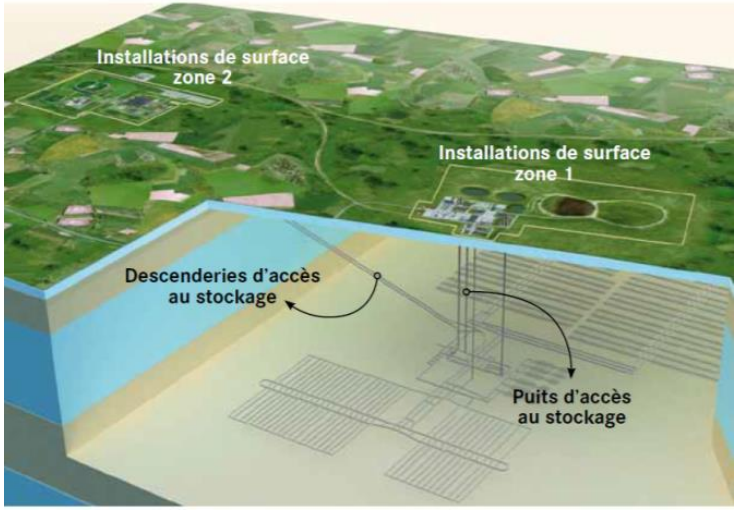
Deep geological disposal

Repository in deep geological media with good confining properties

(Low permeability $K<10^{-12}$ m/s)

Underground structures

= network of galleries



Disposal facility of Cigéo project in France
(Labalette et al., 2013)

Repository phases

Time

Construction
→ Excavation

Maintenance
→ Ventilation

Repository
→ Sealing

Long term
→ Corrosion,
heat generation

Type C wastes (Andra, 2005)

Excavation Damaged Zone (EDZ)

Construction

Mechanical fracturing

Excavation

↓

Stress redistribution

↓

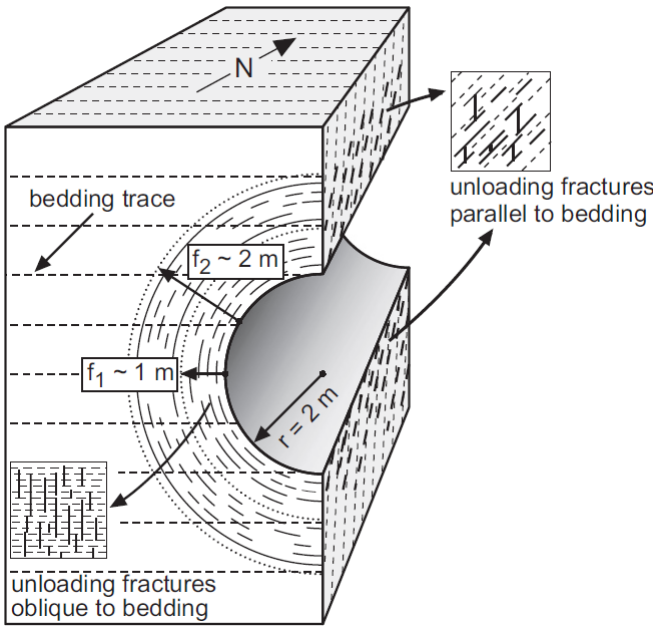
Damage / Fracturing

↓

Coupled processes
HM property modifications

↓

Safety function alteration



Fracturing & permeability increase
(several orders of magnitude)

Opalinus clay in Switzerland
(Bossart et al., 2002)

Maintenance

Water transfer

Galleries ventilation

↓

Air-rock interaction

↓

Drainage / desaturation

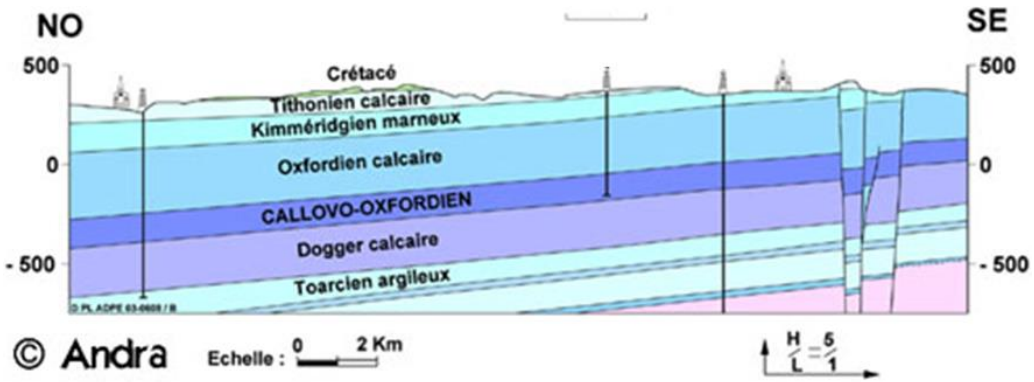
↓

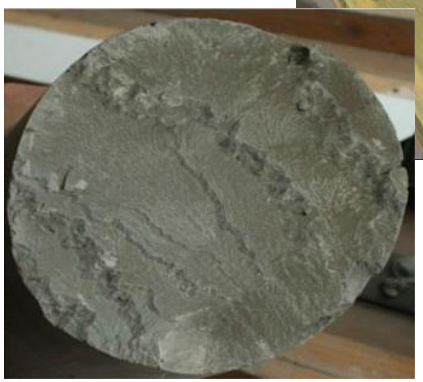
Modification of the
water transfer

Example of EDZ around a cavity

Callovo-Oxfordian claystone (COx)

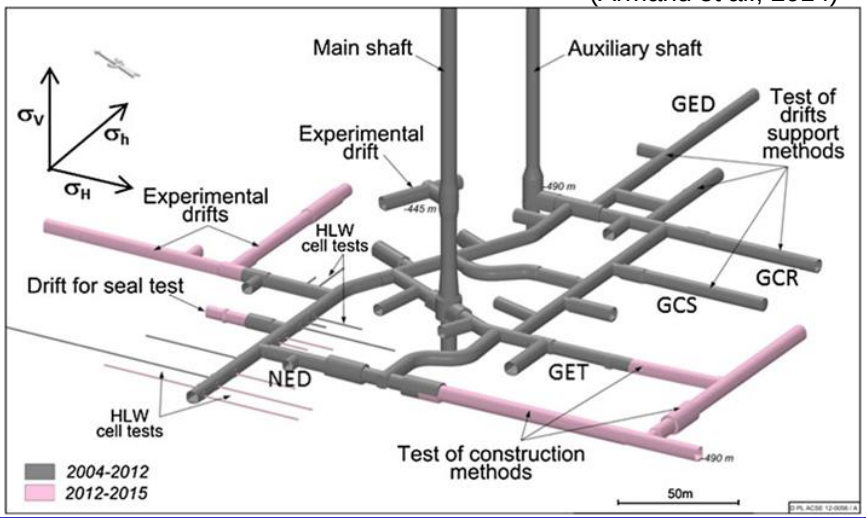
Sedimentary clay rock (France).





Borehole core samples
(Andra, 2005)

(Armand et al., 2014)



- Underground research laboratory

Feasibility of a safe repository

France (Meuse / Haute-Marne, Bure)

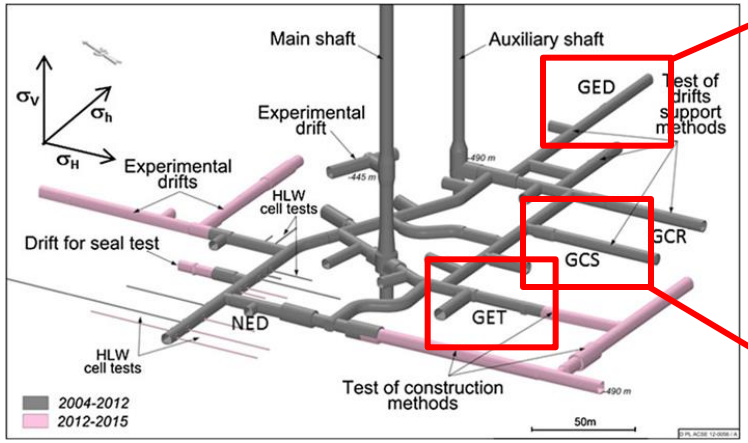
Example of EDZ around a cavity

- Fracturing

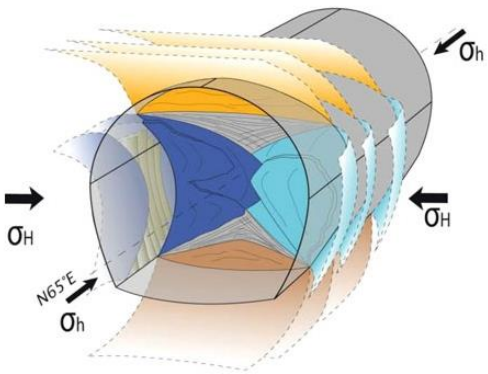
Anisotropies: - stress : $\sigma_H > \sigma_h \sim \sigma_v$

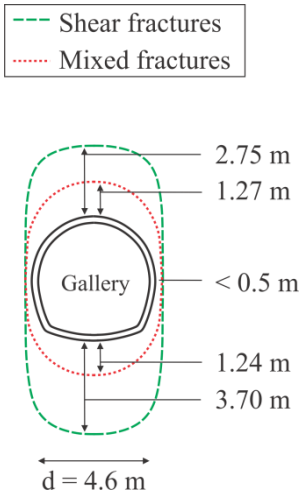
- material : HM cross-anisotropy.

(Armand et al., 2014)

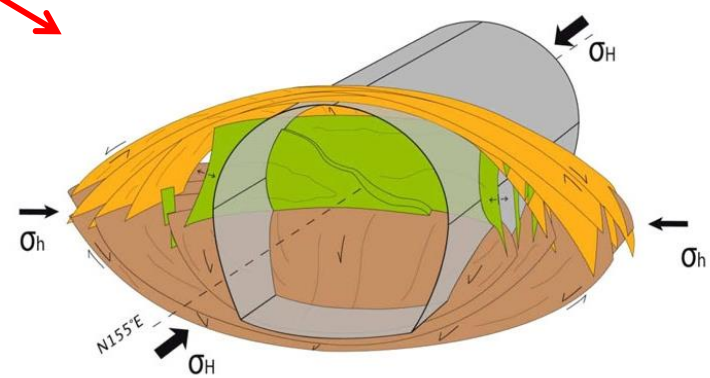


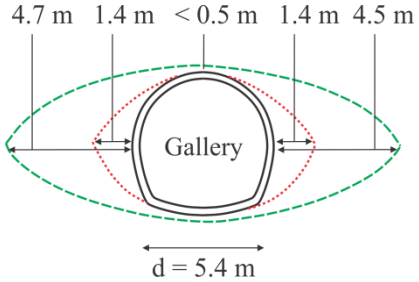
Galery // to σ_h





Galery // to σ_H





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

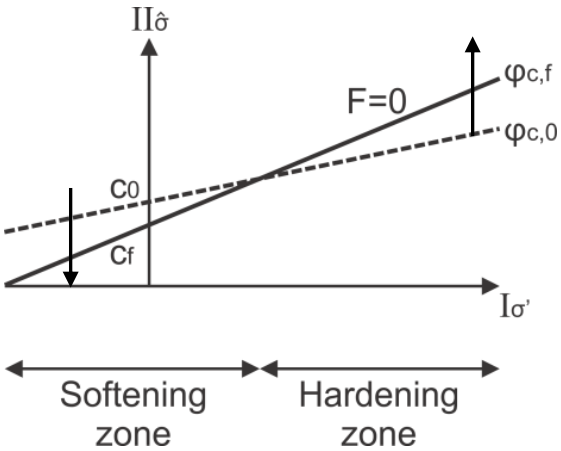
Constitutive models for COx

- Mechanical law - 1st gradient model

Isotropic elasto-plastic internal friction model

Non-associated plasticity, Van Eeckelen yield surface :

$$F \equiv II_{\hat{\sigma}} - m\left(I_{\sigma'} + \frac{3\,c}{\tan\varphi_C} \right) = 0$$



φ hardening / c softening

$$c = c_0 + \frac{\left(c_f - c_0\right)\hat{\varepsilon}^p_{eq}}{B_c + \hat{\varepsilon}^p_{eq}}$$

→ Strain localisation

- Hydraulic law

Fluid mass flow (advection, Darcy) :

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

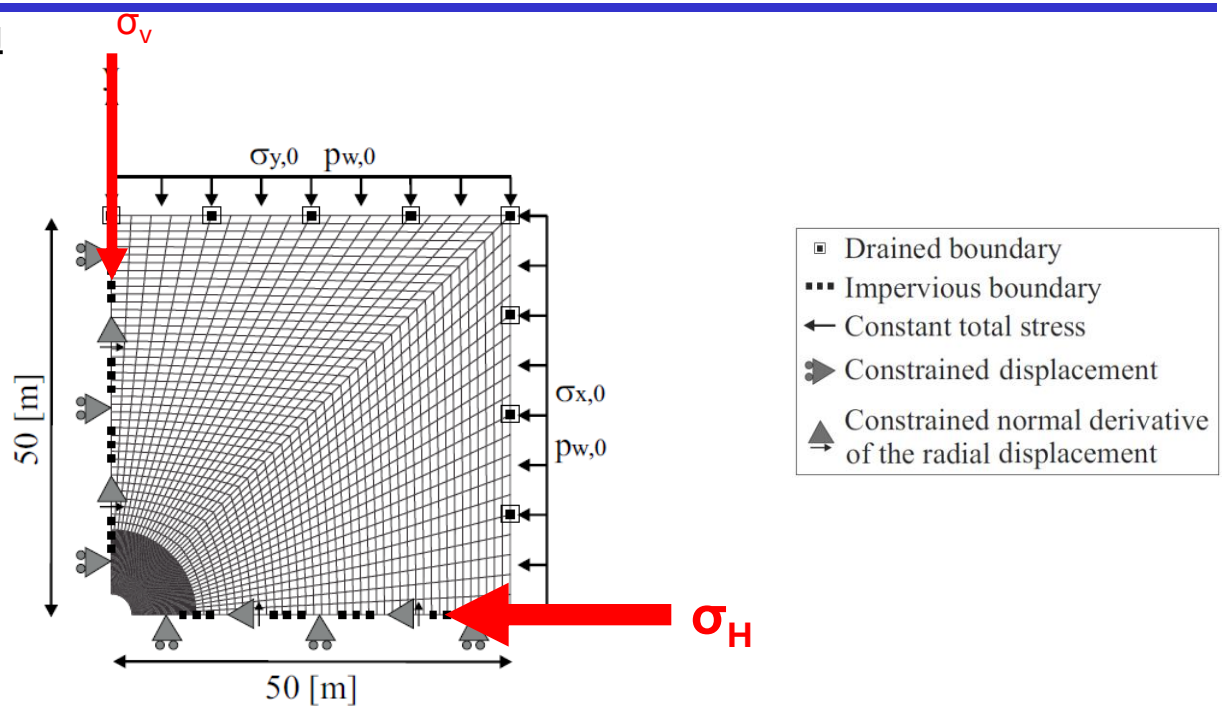
Water retention and permeability curves (Mualem - Van Genuchten's model)

Gallery excavation modelling

- Numerical model

HM modelling in 2D plane strain state

Gallery radius = 2.3 m



- Gallery in COx // σ_h

Effect of stress anisotropy

Anisotropic stress state

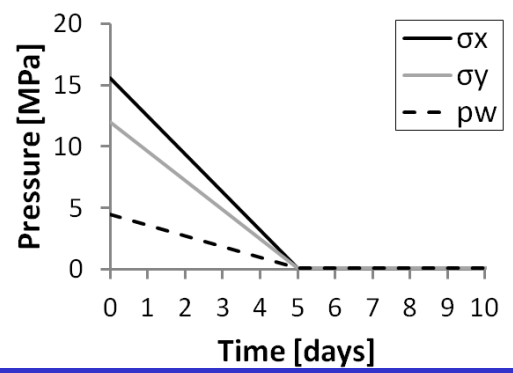
$p_{w,0}$ = 4.5 [MPa]

$\sigma_{x,0} = \sigma_H = 1.3\ \sigma_v$ = 15.6 [MPa]

$\sigma_{y,0} = \sigma_v$ = 12 [MPa]

$\sigma_{z,0} = \sigma_h$ = 12 [MPa]

- Excavation



Example of EDZ around a cavity

- Localisation zone

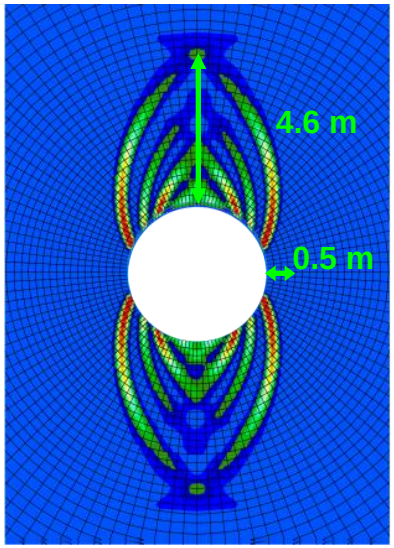
Incompressible solid grains, b=1

Total deviatoric strain

Plasticity

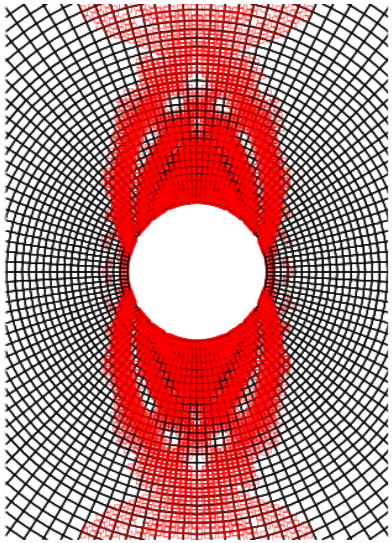
1000 days

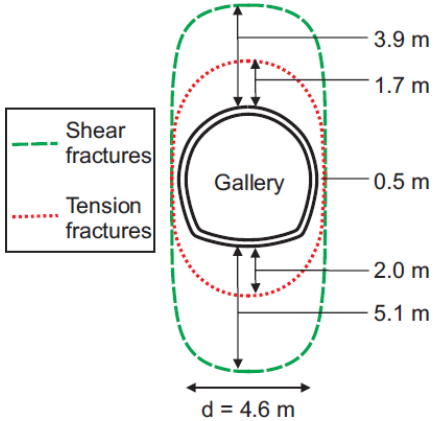
End of excavation



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

0 0.06





→ 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.

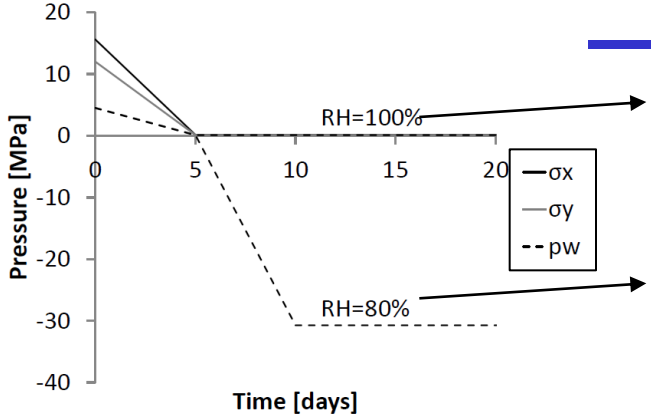
Example of EDZ around a cavity

- 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
$p_w = p_{atm}$ [MPa]

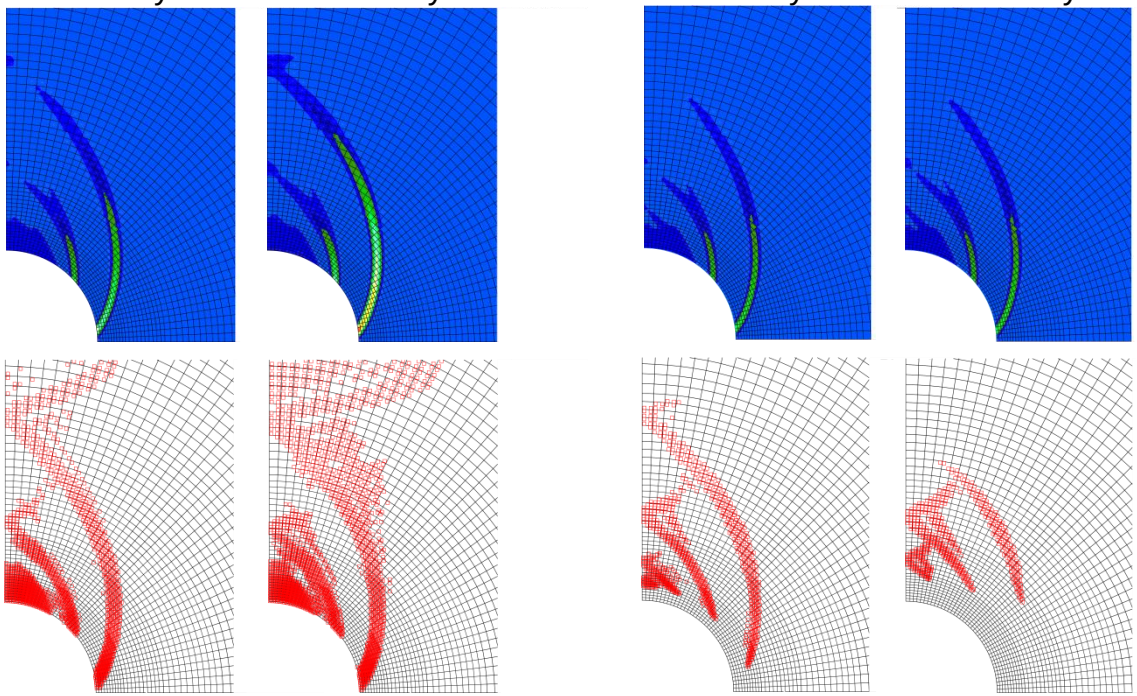
Ventilation
p_w = -30.7 [MPa]

No ventilation | Ventilation

100 days | 1000 days | 100 days | 1000 days

Total deviatoric strain

0 — 0.184



Plasticity

$$\sigma_{ij} = \sigma'_{ij} + b\, S_{r,w}\, p_w\, \delta_{ij}$$

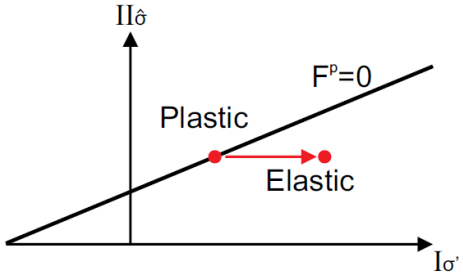
→ suction ↑

→ σ' ↑

→ Elastic unloading

→ Inhibition of localisation

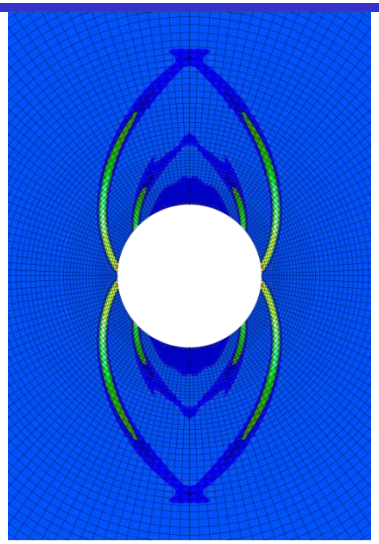
→ Restrain ε

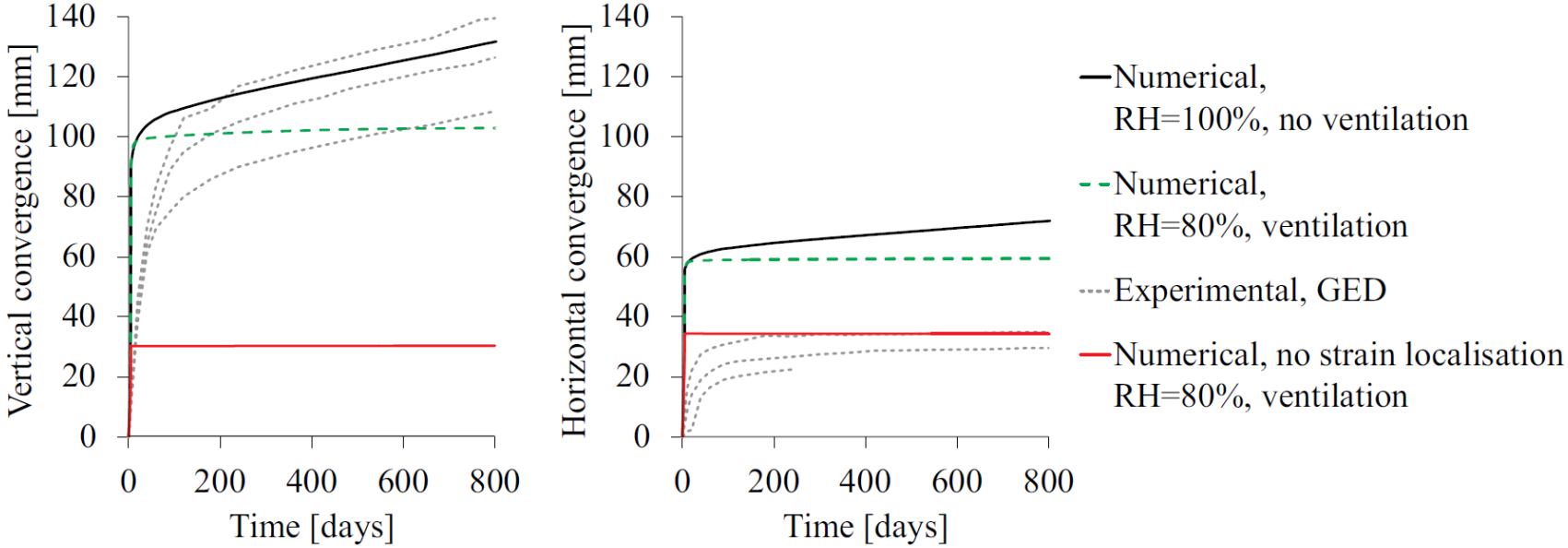


Example of EDZ around a cavity

- Convergence:

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

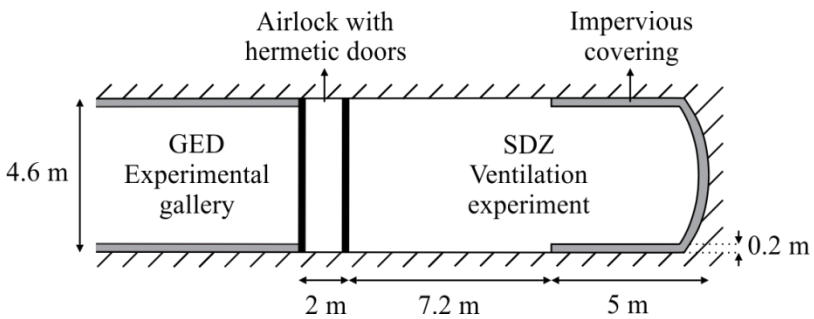


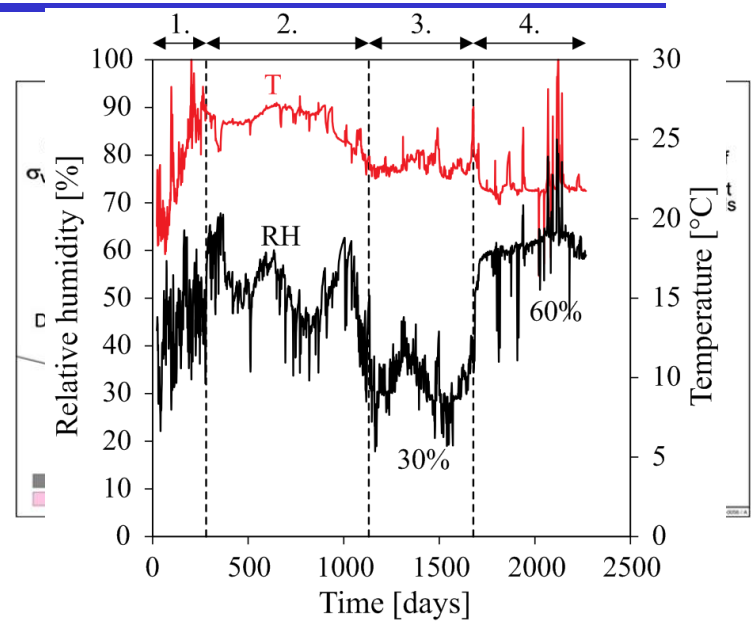


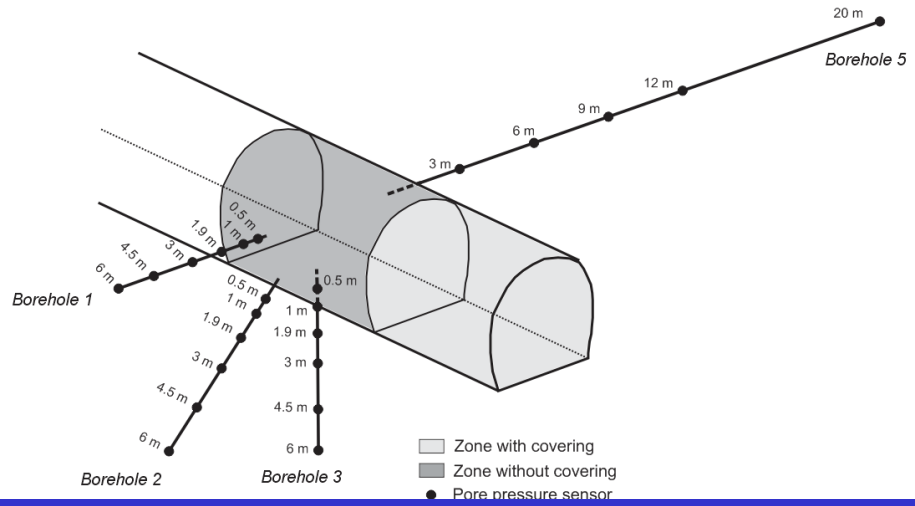
Large-scale experiment of gallery ventilation (SDZ)

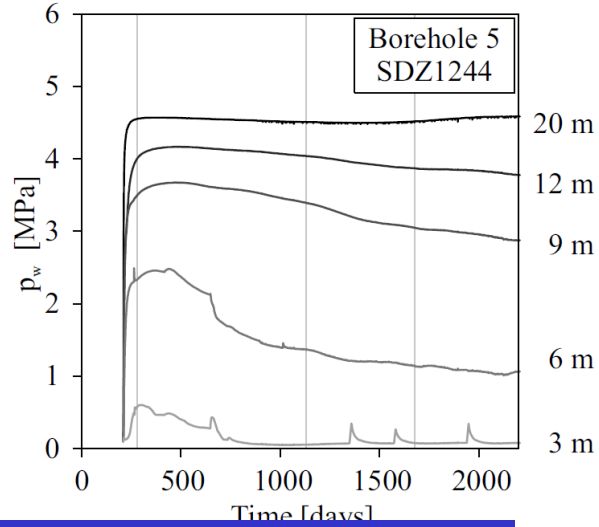
Characterise the effect of gallery ventilation on the hydraulic transfer around it.

→ drainage / desaturation
→ exchange at gallery wall





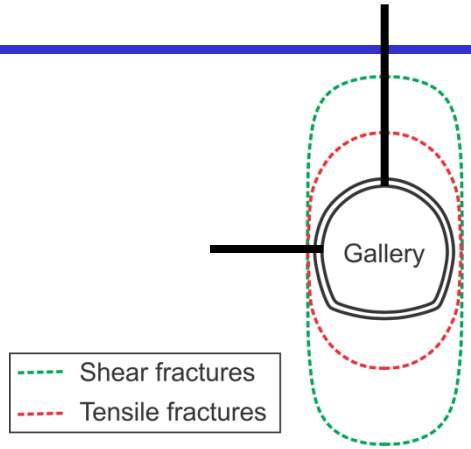


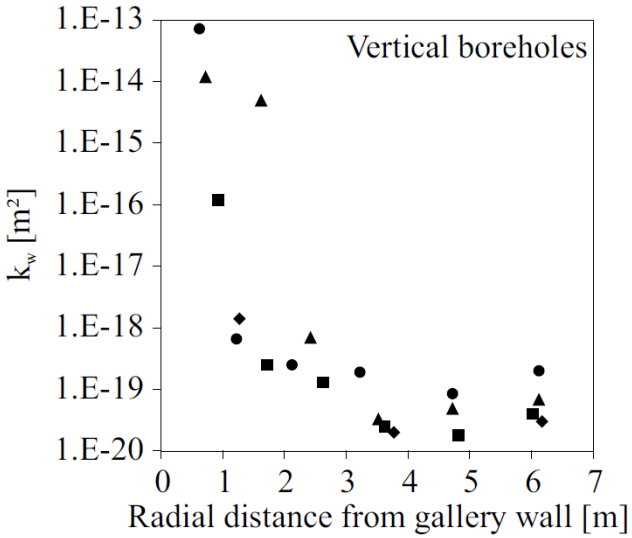


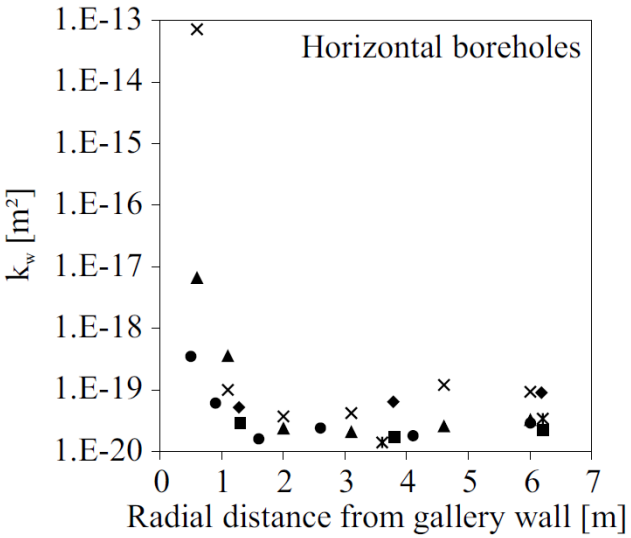
Permeability variation in fractured zone

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

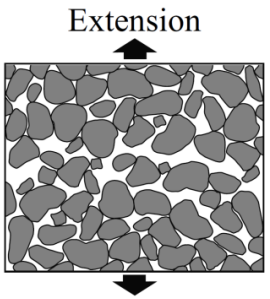
Evolution of intrinsic water permeability

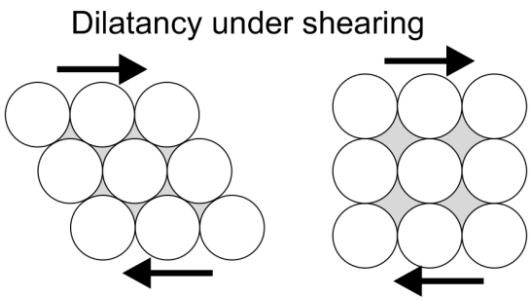
Various approaches: deformation, damage, cracks…

- Relation to deformation

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

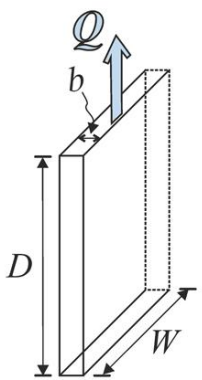
$$k_w = k_{w,0} \frac{(1-\phi_0)^{\xi_1}}{\phi_0^{\xi_2}} \frac{\phi^{\xi_2}}{(1-\phi)^{\xi_1}} \qquad \varepsilon_v = \frac{\varepsilon_{ii}}{3}$$



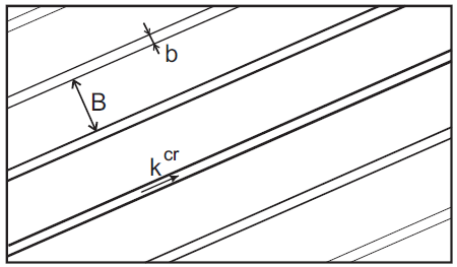


- Fracture permeability

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



$$k_w^{cr} = \frac{b^2}{12}$$



$$k_w = \frac{b^3}{12B}$$

$$b = b_0 + B\left\langle \varepsilon^n - \varepsilon_0^n \right\rangle$$

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

Localised deformation
Fracture initiation

- Empirical law

Related to strain localisation effect
Permeability variation threshold

$$k_{w,ij} = k_{w,ij,0}\left(1 + \beta_{per}\left\langle YI - YI^{thr}\right\rangle \hat{\varepsilon}_{eq}^{\,3}\right) \qquad YI = \frac{II_{\hat{\sigma}}}{II_{\hat{\sigma}}^{p}}$$

Modelling of excavation and SDZ experiment

HM coupling in EDZ

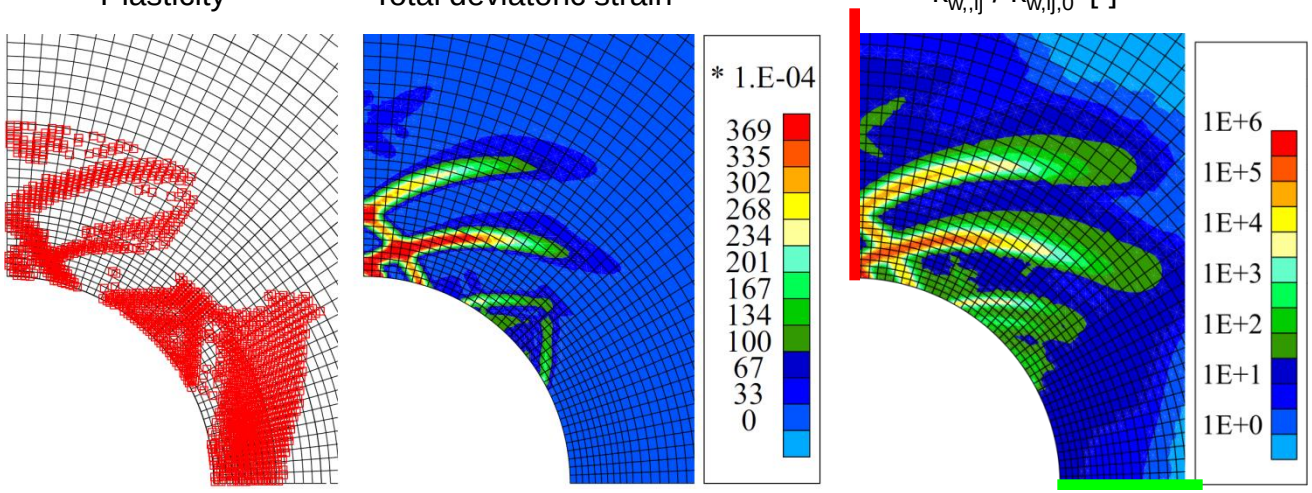
- Gallery excavation

SDZ → GED gallery // σ_h

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

→ Localisation zone dominated by stress anisotropy

Plasticity | Total deviatoric strain | $k_{w,,ij} / k_{w,ij,0}$ [-]

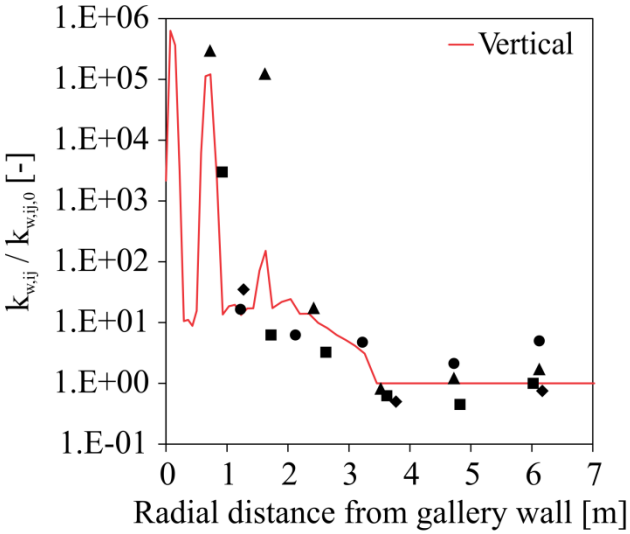


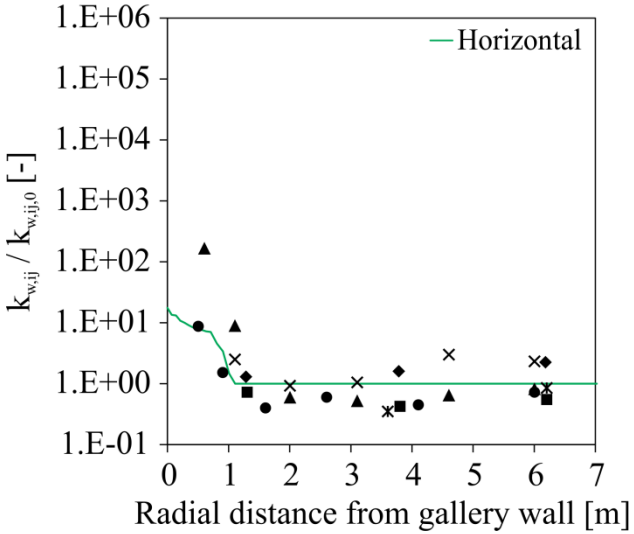
- Intrinsic permeability evolution

$$\frac{k_{w,ij}}{k_{w,ij,0}} = \left(1 + \beta \left\langle YI - YI^{thr} \right\rangle \hat{\varepsilon}_{eq}^{\,3}\right)$$

$$YI^{thr} = 0.95$$

Cross-sections





Plastic strain and a part of the elastic one → EDZ extension + k_w increase

Modelling of the SDZ experiment

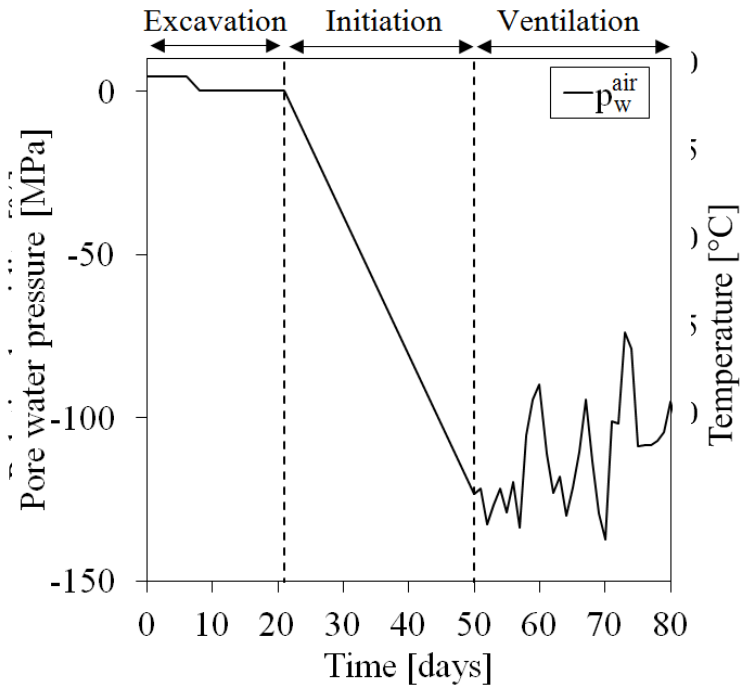
- Water pressure in the cavity air

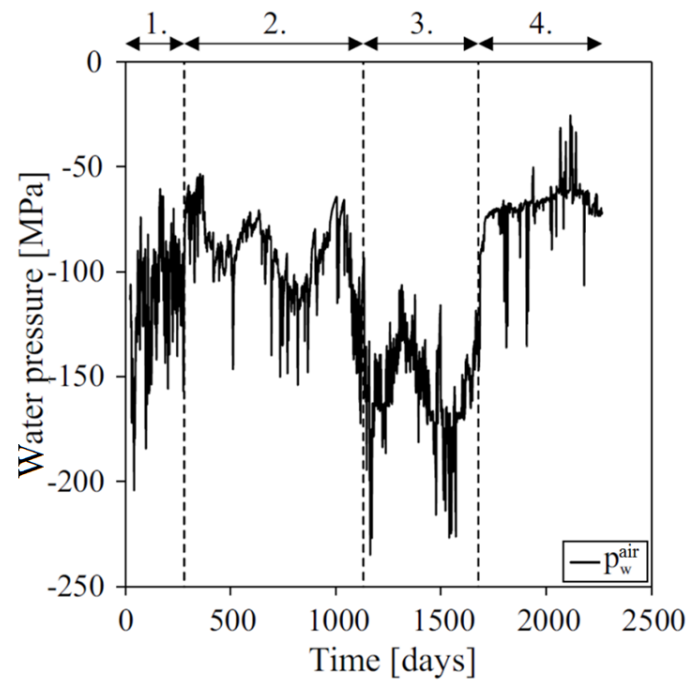
p_w (suction) corresponding to RH and T (Kelvin's law).

$$p_w^{air} = \frac{\rho_w RT}{M_v} \ln(RH) + p_{atm} \qquad \rho_v^{air} = RH\ \rho_v^0$$

Imposed at gallery wall through hydraulic boundary condition.

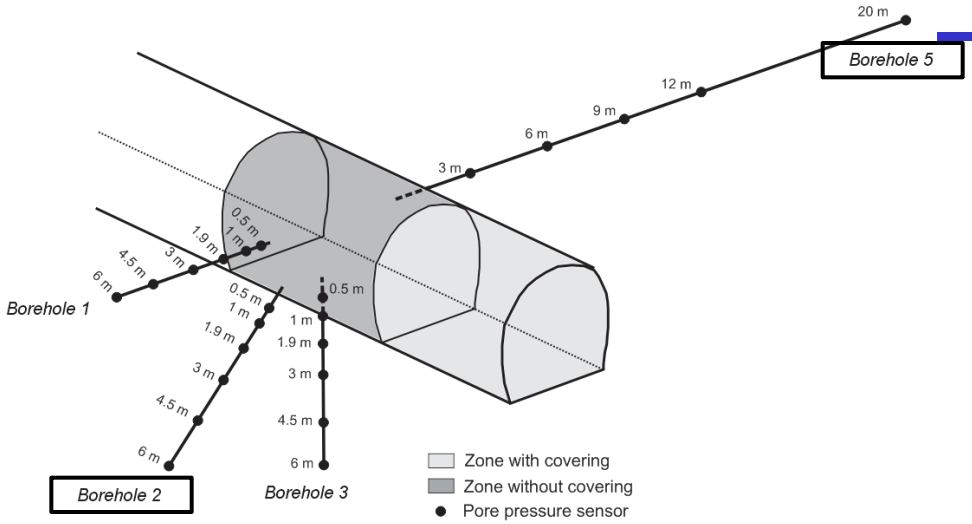
Excavation (RH=100%) → Initiation phase → Ventilation



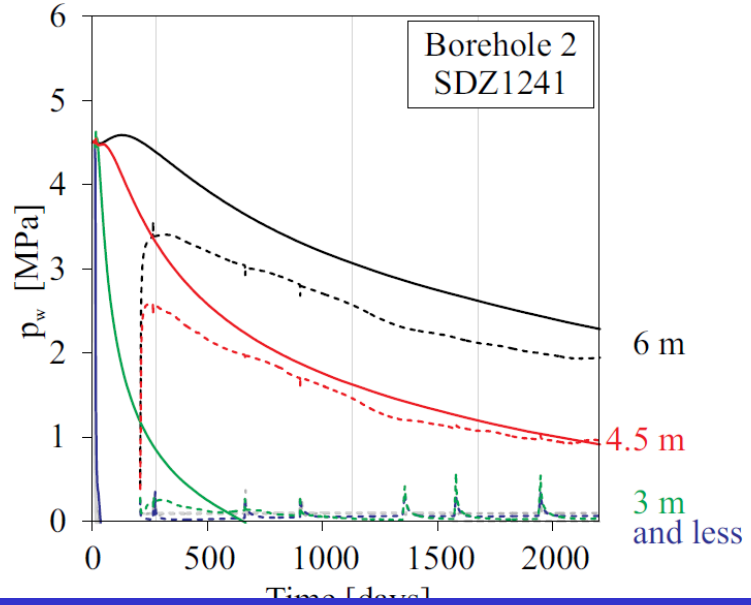


Example of EDZ around a cavity

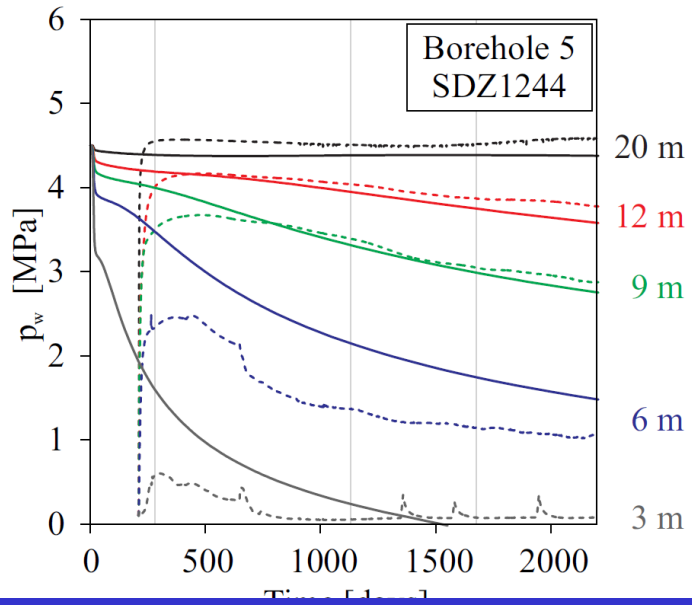
- Drainage / p_w reproduction



Oblique 45°



Horizontal



Experimental

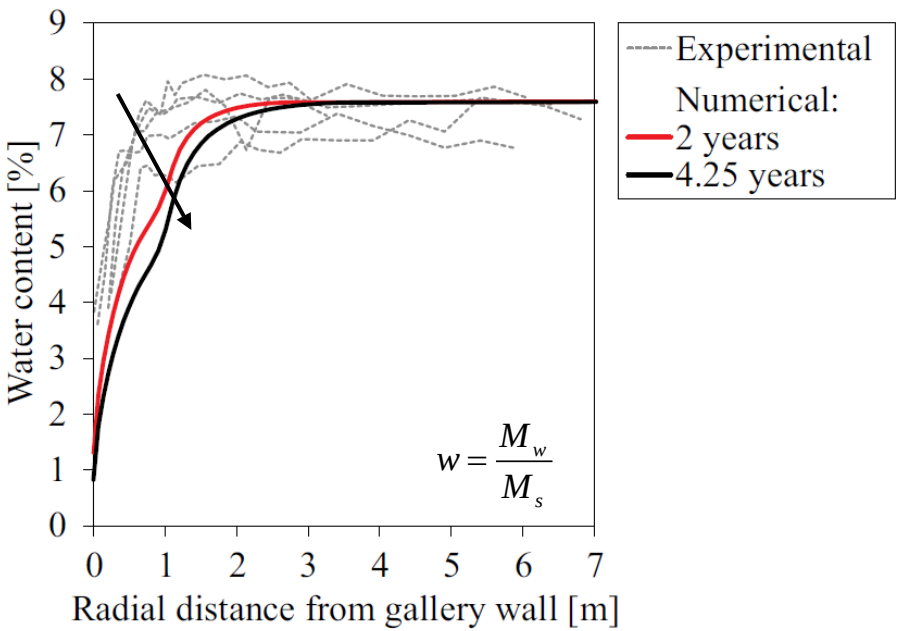
Numerical

$\alpha_v = 10^{-3}$ m/s

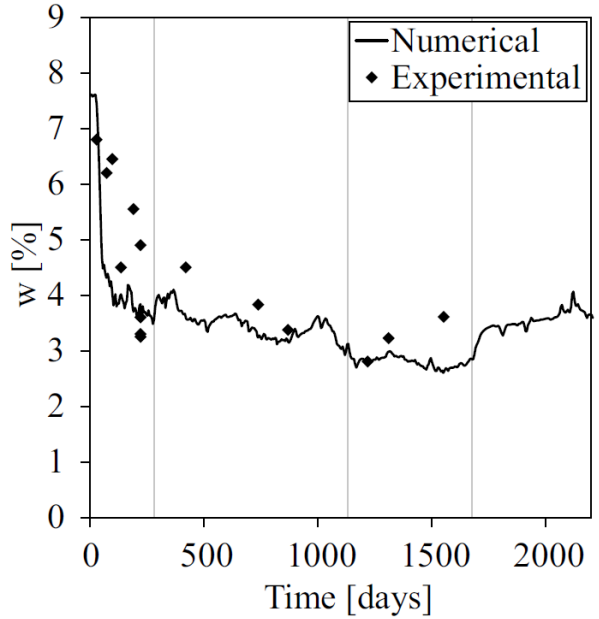
Example of EDZ around a cavity

- Desaturation EDZ / w reproduction

Horizontal boreholes



At gallery wall



→ Desaturation: overestimation in long term

→ Vapour transfer ($\alpha_v = 10^{-3}$ m/s)

→ Good reproduction at gallery wall

Outline:

- *Introduction*
- *Theoretical tools*
- *Numerical models*
- *Numerical application*
- *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.