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FEM-DEM Multiscale analysis in Geomechanics : Strain Localisation and 2nd Gradient Regularisation

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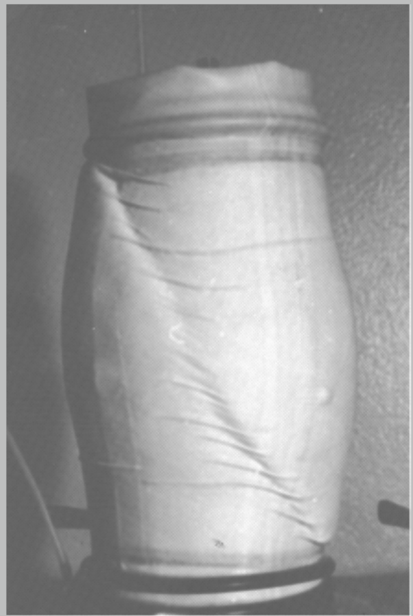
Outline

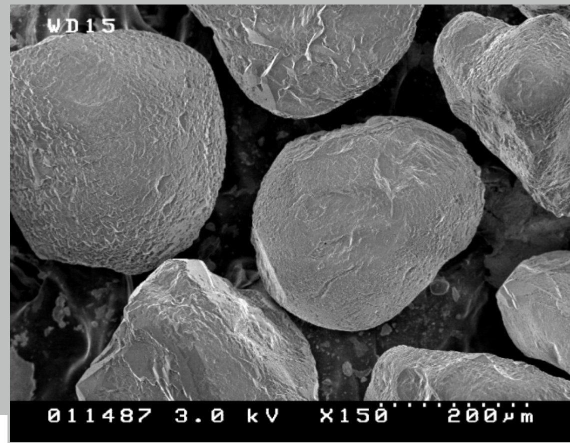
1. Introduction & principle
2. Micro-scale (DEM) Model
3. Multi-scale Coupling Method
4. FEM-DEM simulation
5. 2nd gradient : motivation, methods and results
6. Conclusions & Perspectives

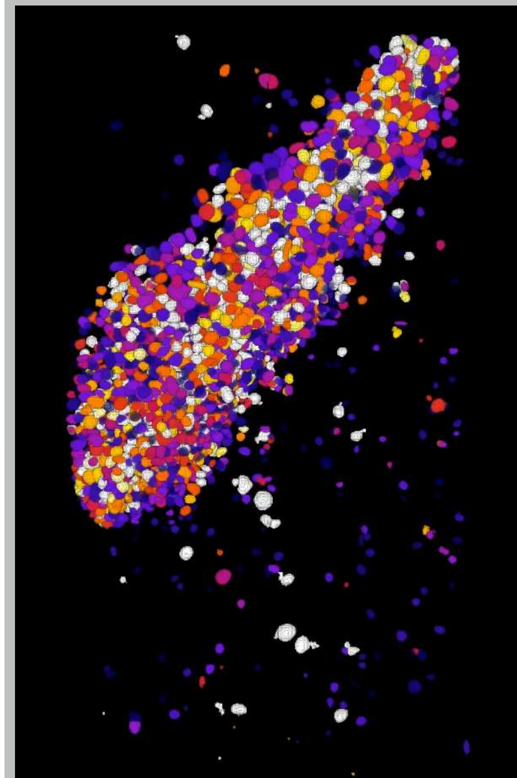
Introduction : bridging scales in Geomechanics :



in experiments ...

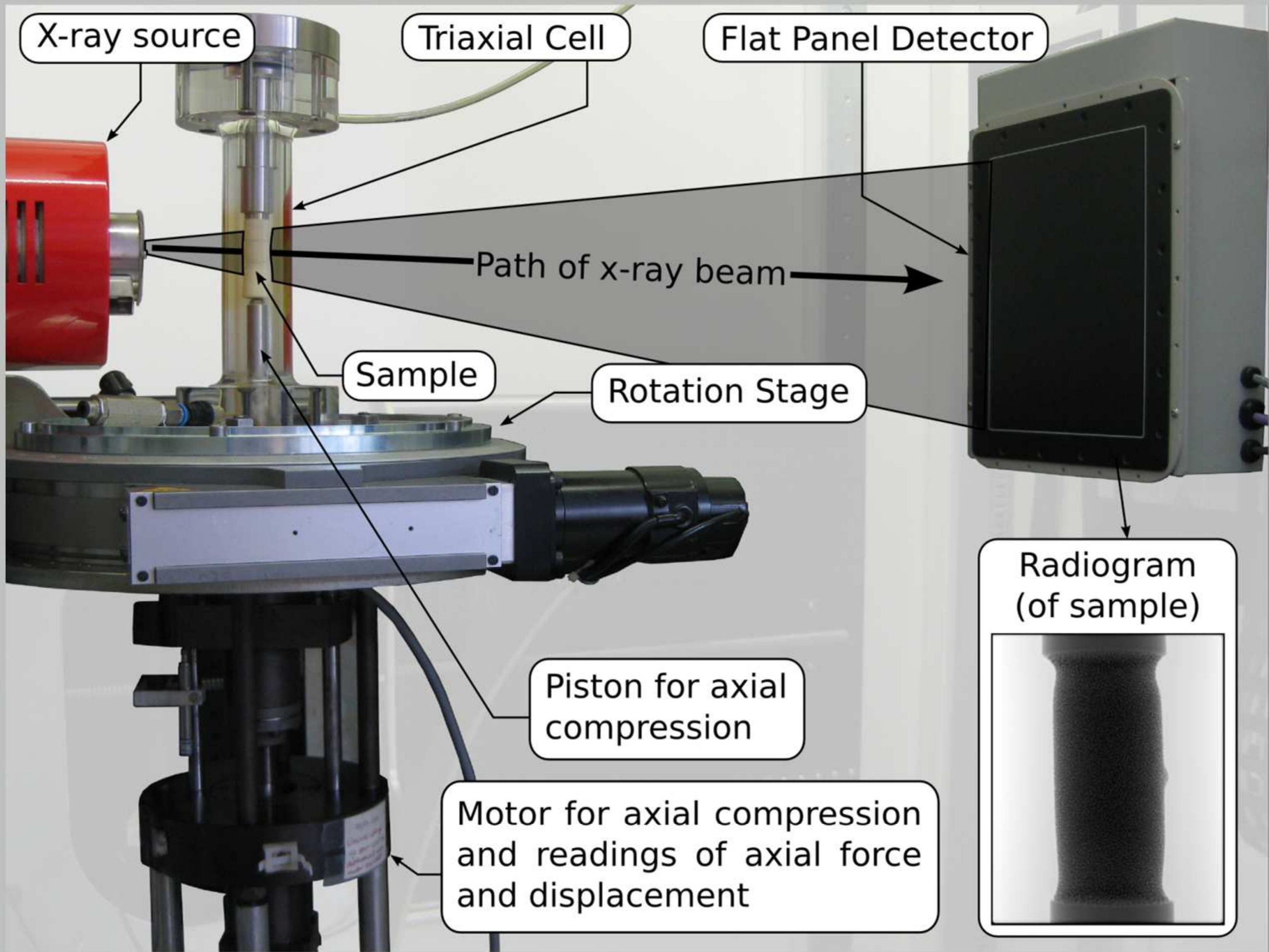
?





In experiments :
X-Ray µtomography allows to catch both the big picture and the fine details in a single shot

In-situ triaxial test in sand using X-Ray tomography



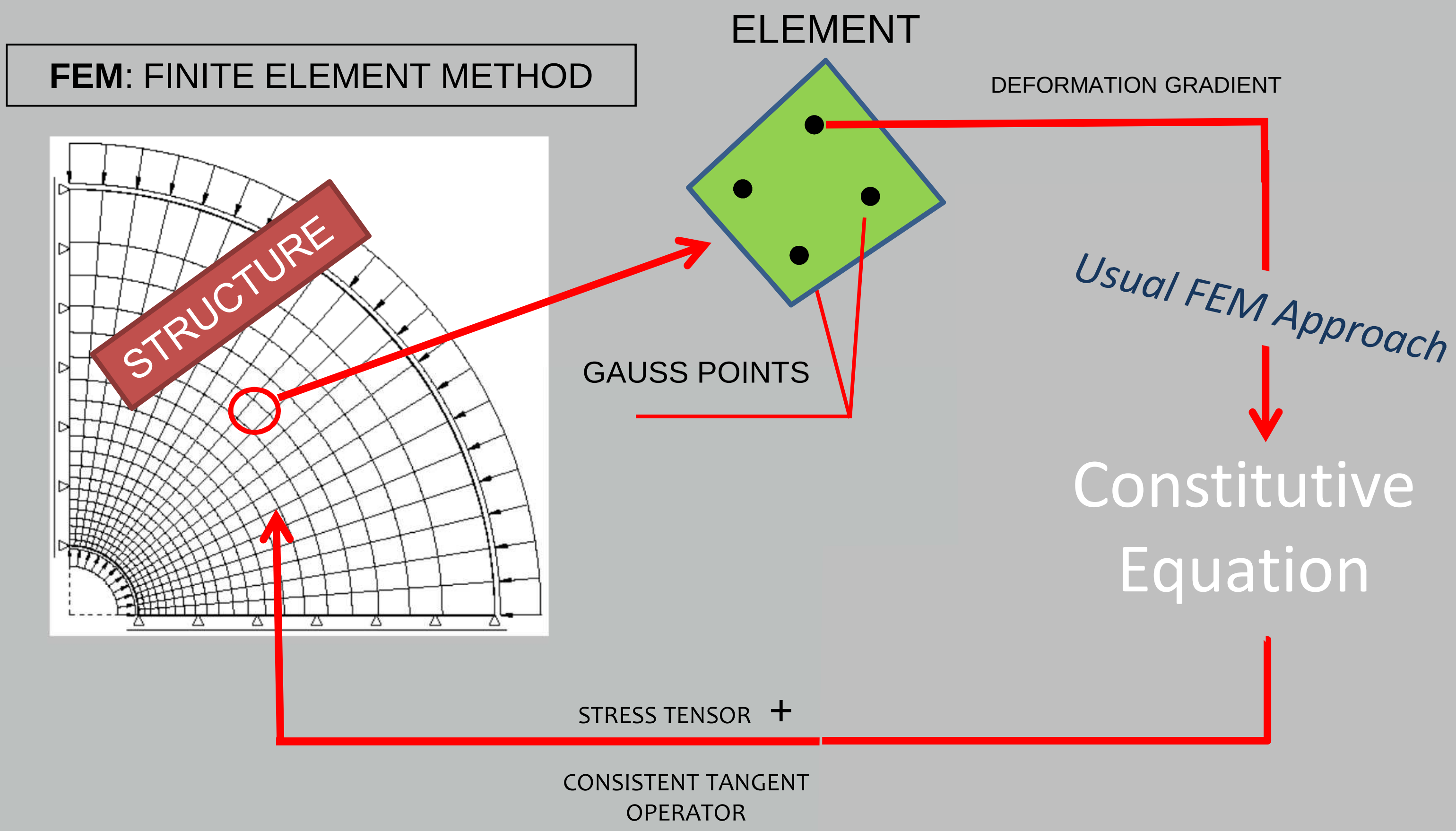
Introduction : bridging scales in Geomechanics : **modelling**

→ **A continuum media**
or
an assembly of particles ?

Continuum : FEM	Particles : DEM
☺ well suited to Real scale problem ☹ CAN NOT realistically model their discrete nature	☺ Reproduces « naturally » the complex behaviour of grains assembly : cyclic response, anisotropy, strain path dependency ☹ Computation time depends on the number of grains -> high CPU costs > limitation to small problems
→ **Coupling FEM-DEM** ☺ ☺	

Principle

Introducing a two-scale numerical homogenization approach by FEM - DEM



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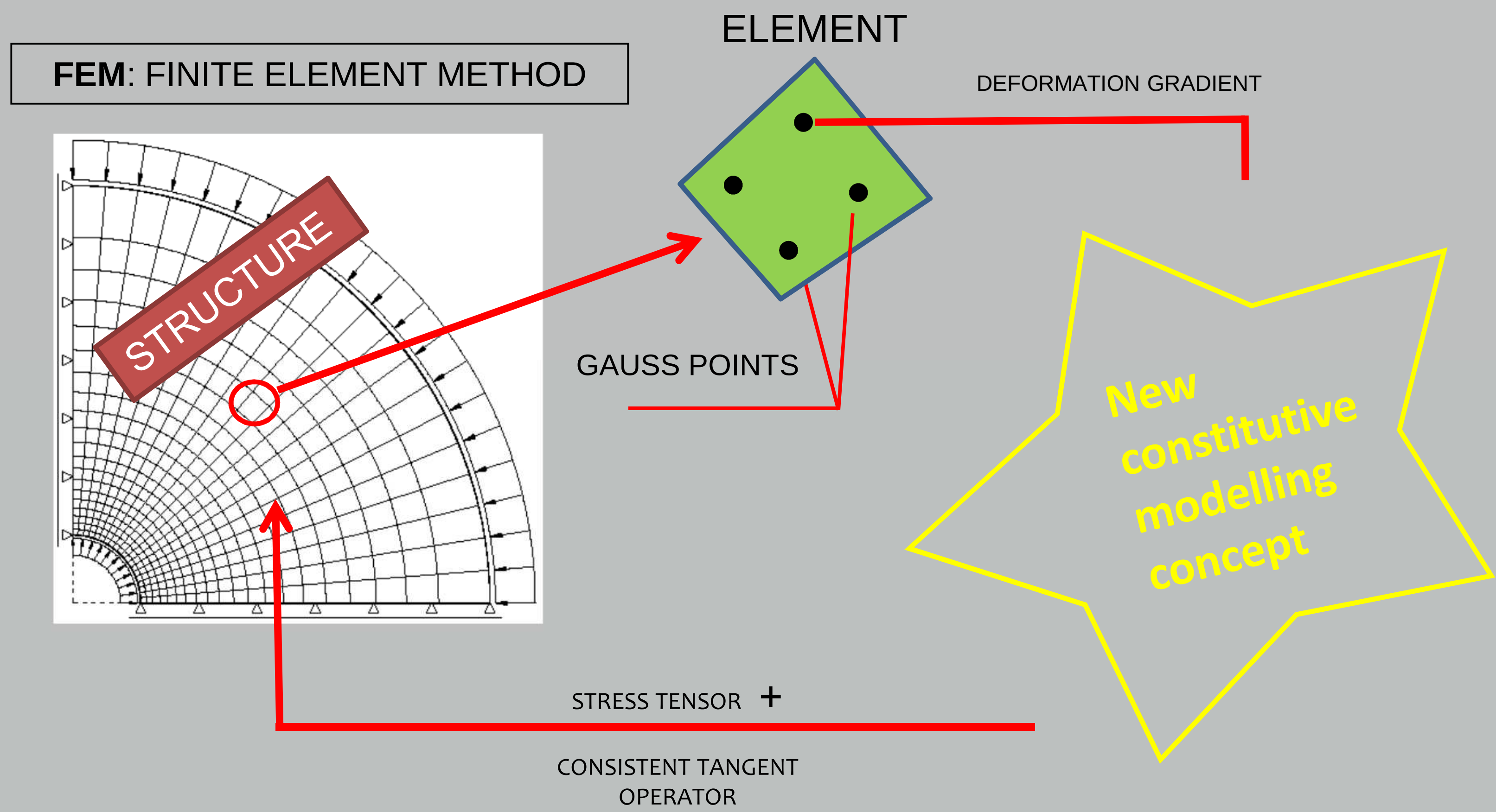
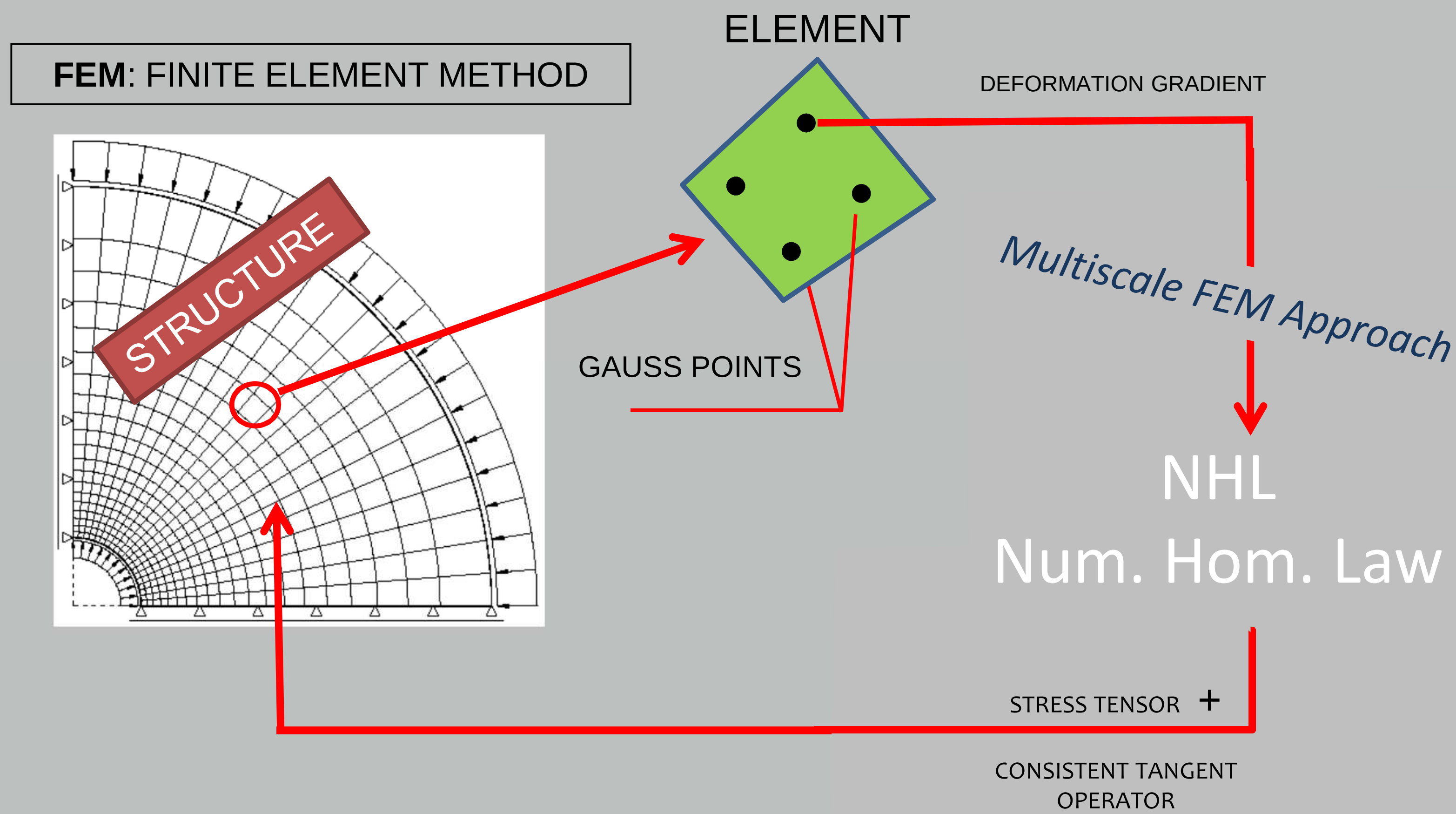


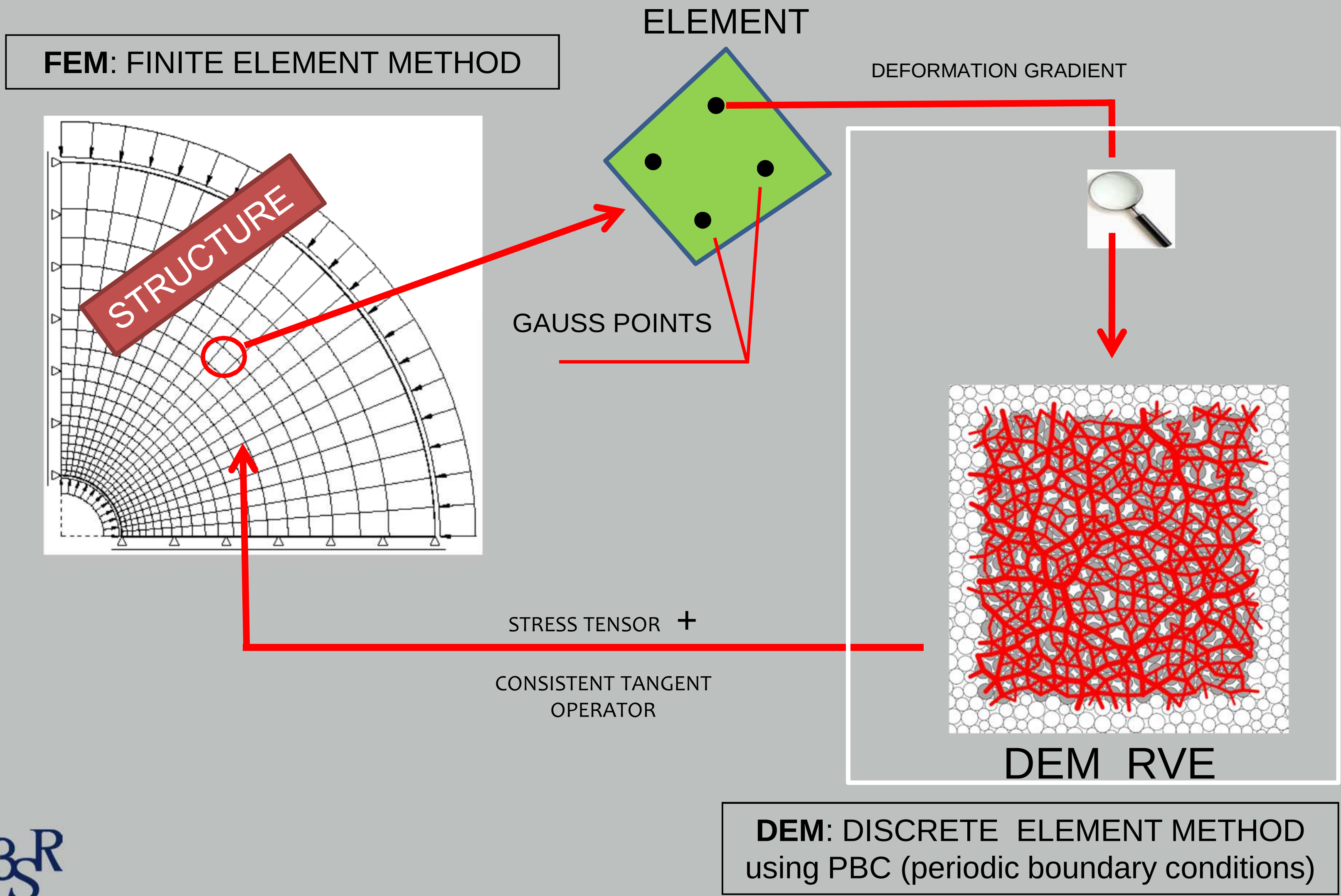
Principle

Introducing a two-scale numerical homogenization approach by FEM - DEM



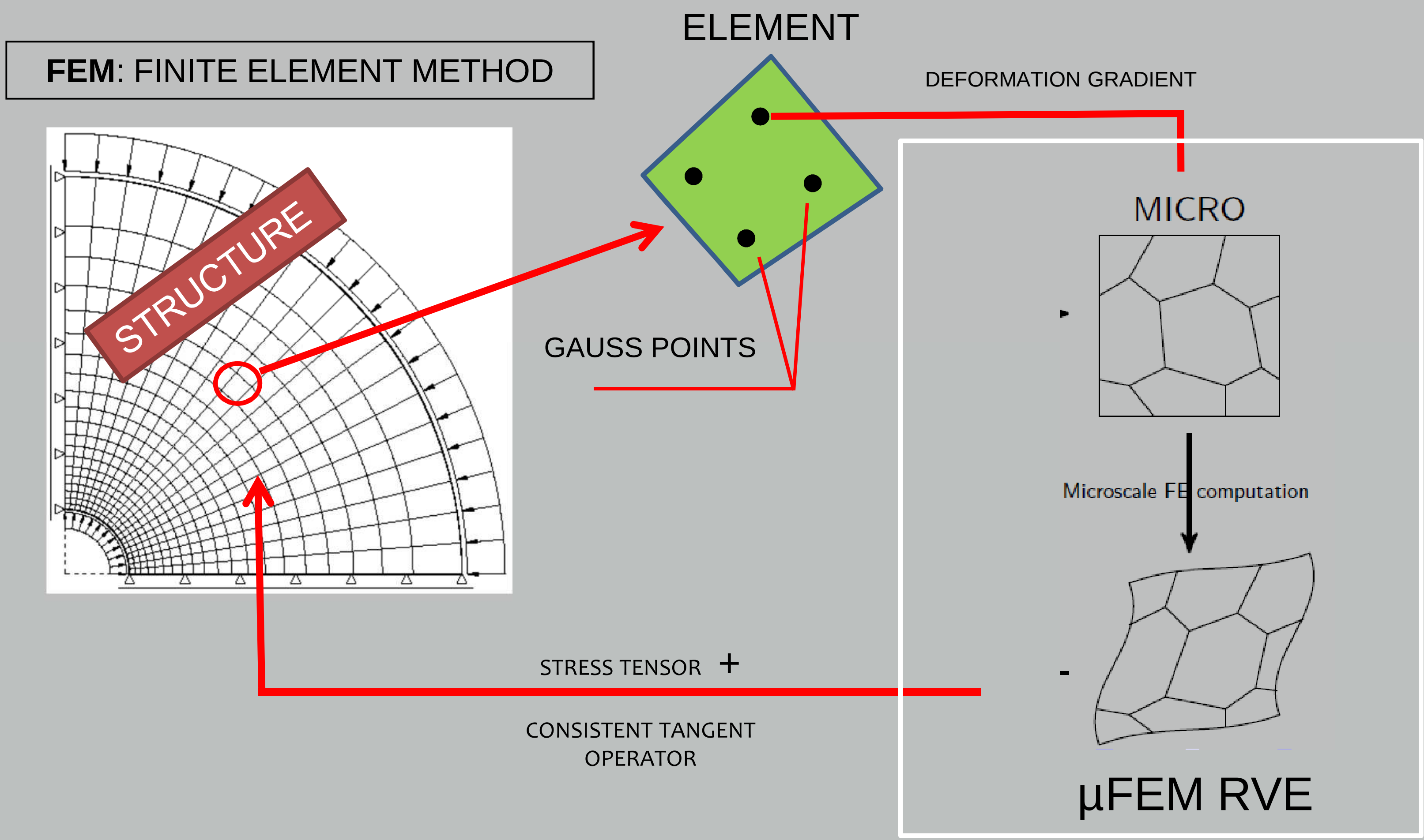
Principle FEM x DEM

A two-scale numerical homogenization approach by FEM - DEM



Principle FEM^2

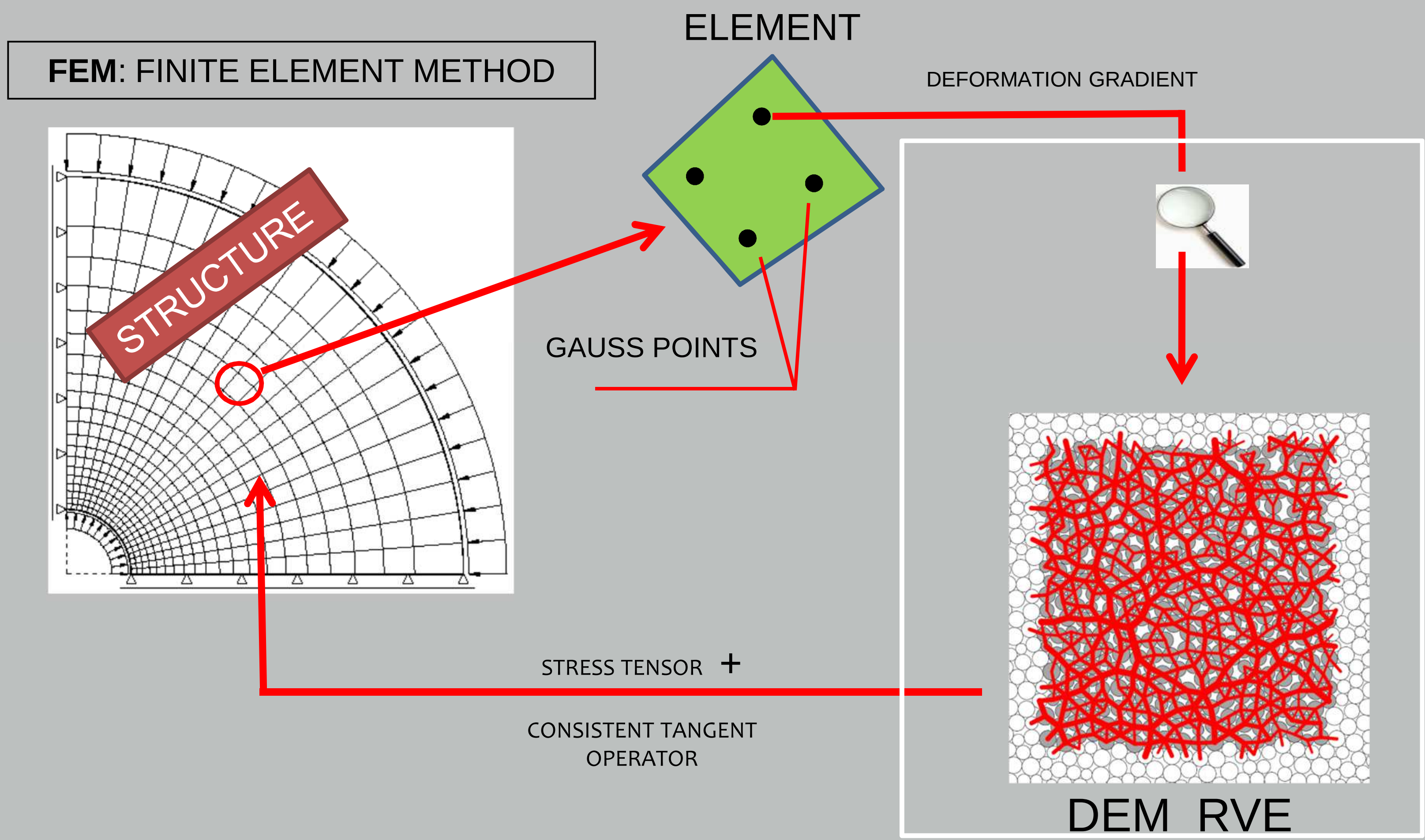
A two-scale numerical homogenization approach by FEM - DEM



µFEM: FINITE ELEMENT METHOD
using PBC (periodic boundary conditions)

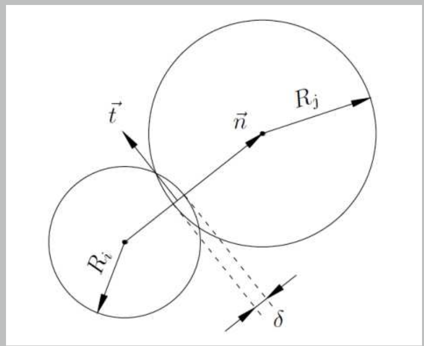
Principle FEM x DEM

A two-scale numerical homogenization approach by FEM - DEM

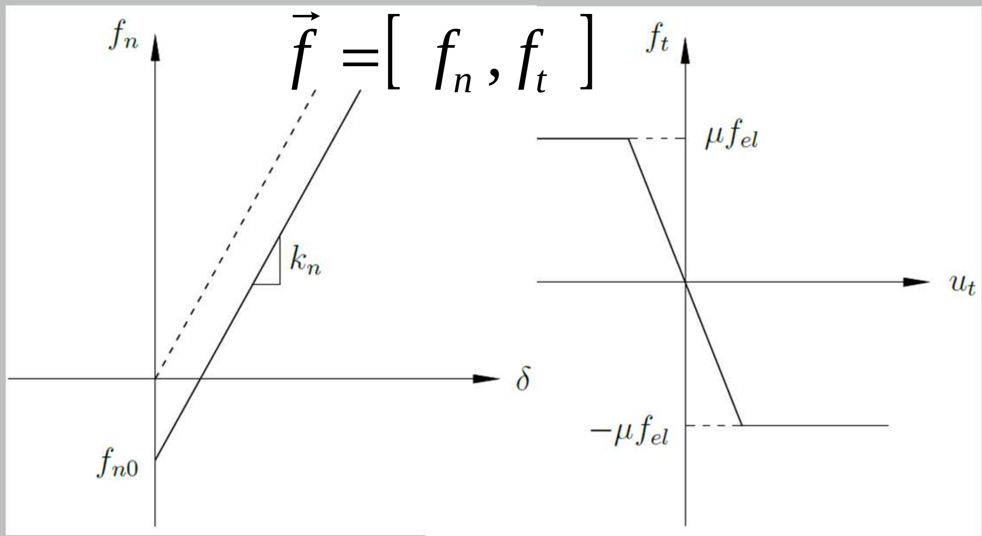


DEM: DISCRETE ELEMENT METHOD using PBC (periodic boundary conditions)

Micro-scale Model



Discrete **E**lement **M**ethod
(Soft contact dynamics type, Cundall & Strack 1979)
with bi-**P**eriodic **B**oundary **C**onditions



Macrosc. Stress tensor :

$$\sigma_{ij} = \frac{1}{S} . \sum_{k=1}^{N_C} f_i^k \cdot l_j^k$$

Contact laws *

- Normal repulsive contact force

$$f_{el} = k_n \cdot \delta$$

$$\begin{cases} \delta > 0 & \text{Contact present} \\ \delta = 0 & \text{No contact} \end{cases}$$

- Tangential contact force

$$\delta f_t = k_t \cdot \delta u_t$$

- Coulomb condition

$$\| f_t \| \leq \mu . f_{el}$$

- Cohesion

$$f_n = f_{el} + f_{n0}$$

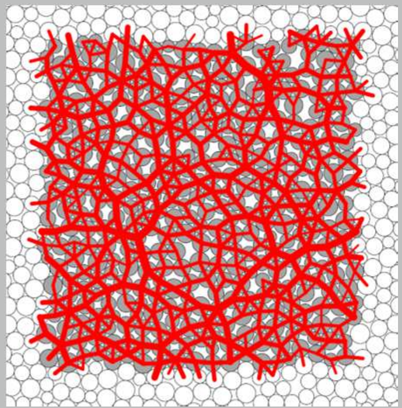
f_{n0} : cohesive force

$$f_{n0} = p^* . \sigma_0 \qquad p^* = 1,2,\ldots$$

* : (e.g. Gilabert et al., 2007)

Micro-scale Model

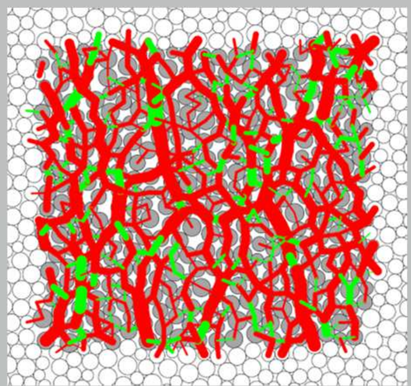
Biaxial test (DEM with PBC): REV contains 400 particles



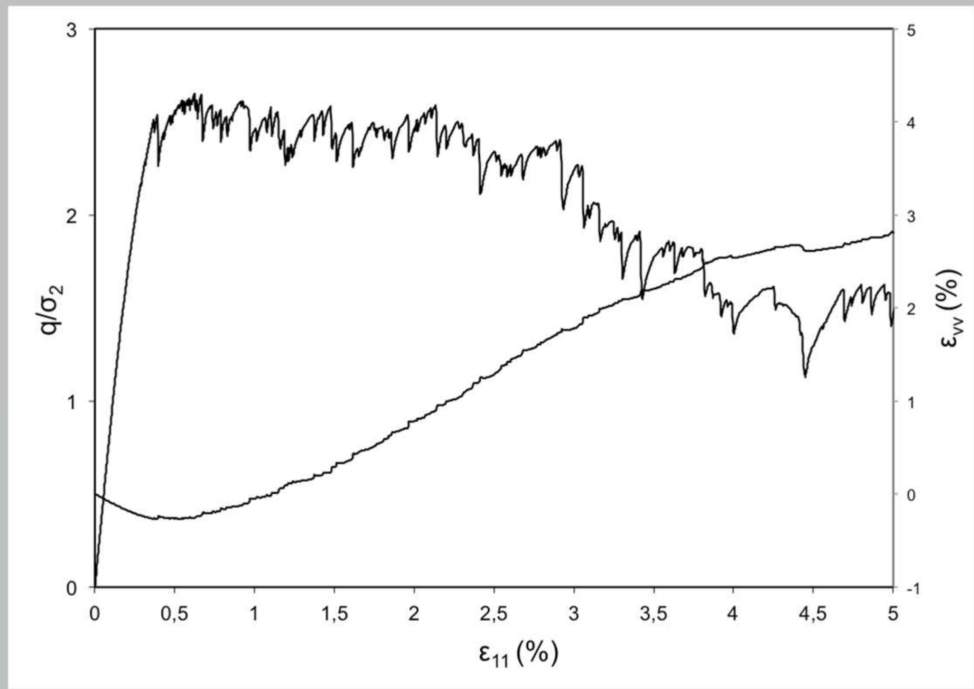
Initial configuration

f_c effective

$f_c = 0$

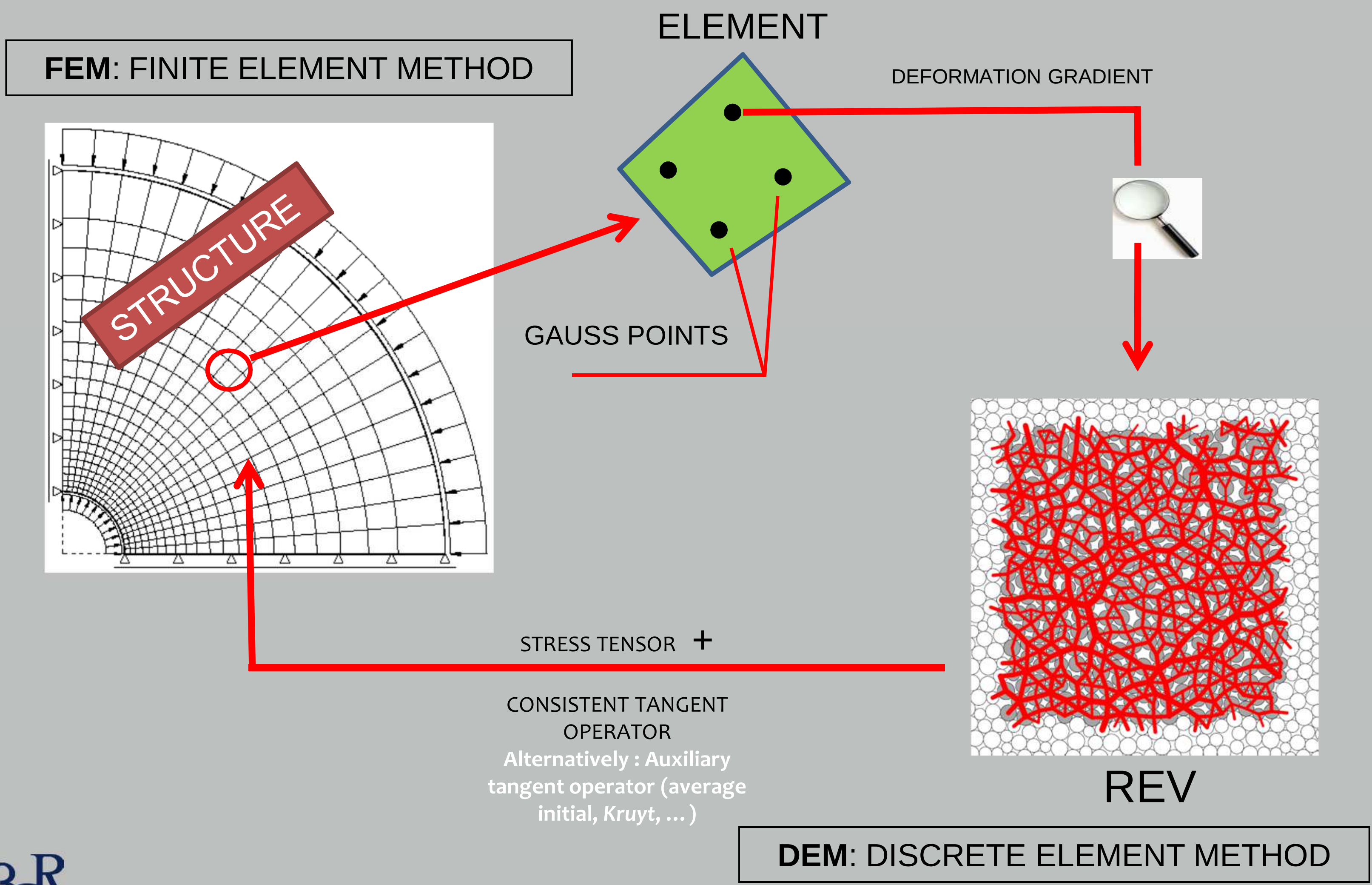


at 3% of axial strain (ε_{11})



Principle

A two-scale numerical homogenization approach by FEM - DEM



Principle

What do we need ? a **FEM code** + a **DEM code** + a **bridging procedure**

- **FEM code :**
  the choice made has been to use the large multi-purpose FEM code Lagamine[1], Liège University (ULg). Also implemented in FlagShyp[2]
- **DEM code** : an as-compact-as-possible DEM kernel !
  -> in-house 3SR-Grenoble DEM code, Geomechanics team.
  strong requirement : quasi-perfect static equilibrium
  at the end of each DEM step.
- **Bridge :**
  direct incorporation of the DEM code as a constitutive law in the FEM code (convenient for sequential programming, or OpenMP parallel programming)

1 – Lagamine, Liège University Ulg
2 – FlagShyp Software, Bonet and Wood, Swansea UK 2012

Two examples of failure in real geomaterias

1. **Triaxial test :**

ideally, should be *homogeneous*, but …

in the lab, observation :

localised deformation

Triaxial test on Hostun sand specimen, JL Colliat, 3SR Grenoble 1986

2. **Borehole or gallery stability problem ,**

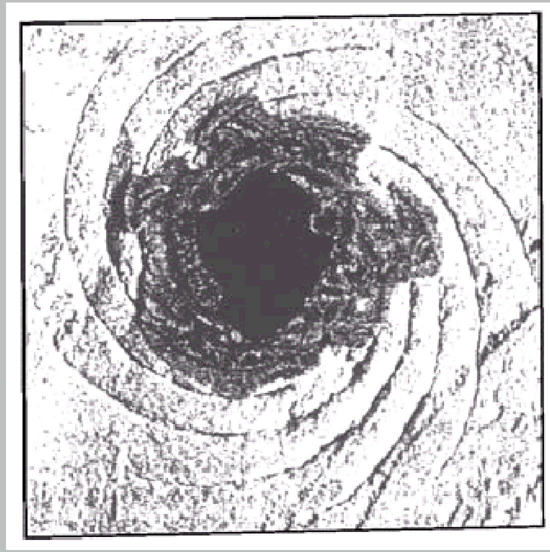
(can be studied as a hollow cylinder under differential pressure)

(analogous to a borehole or a gallery)

heterogeneous by essence

in the field, observation :

localised deformation



van den Hoek, P.J., Smit, D.-J., Kooijman, A.P., de Bree, P., Kenter, C.J., Khodaverdian, M., 1994. Size dependancy of hollow-cylinder stability. Eurock, vol. 94. Balkema, Rotterdam.

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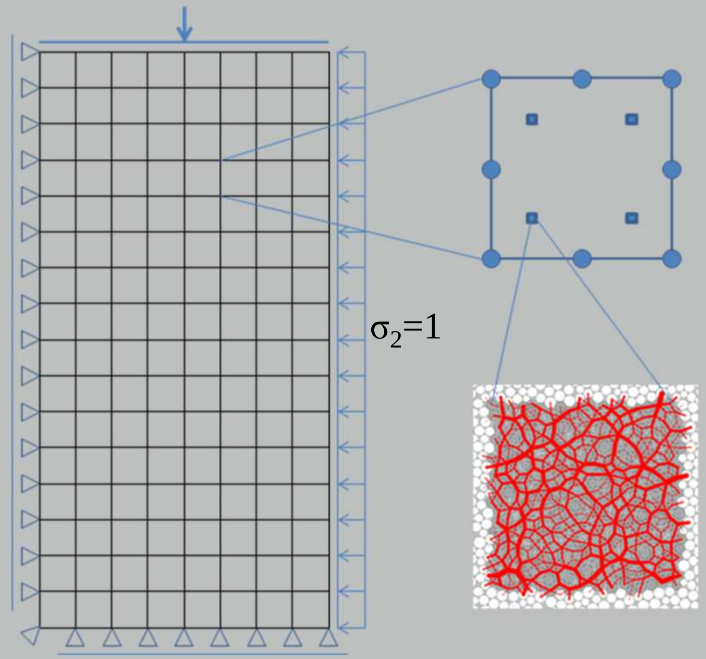
Multiscale Computations: Numerical results



FEM x DEM simulation of a biaxial compression test

DEM parameters

$$\kappa = k_n / \sigma_0 = 1000$$

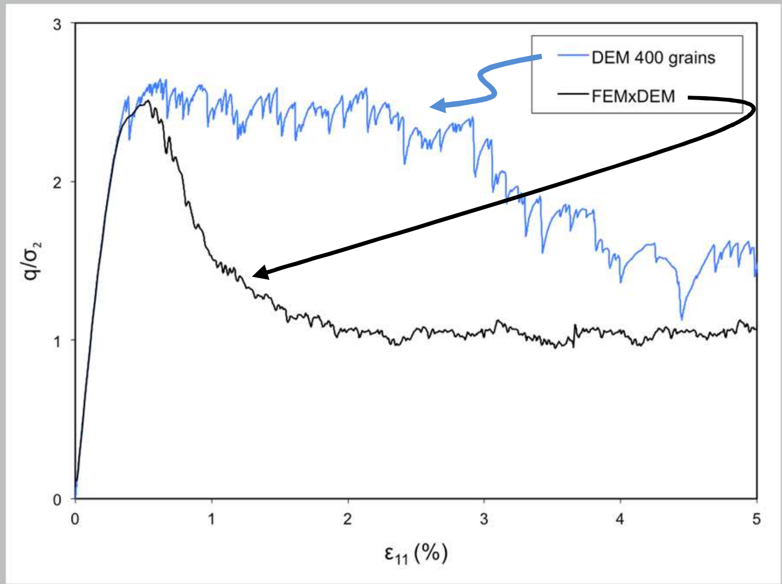
$$k_n / k_t = 1$$

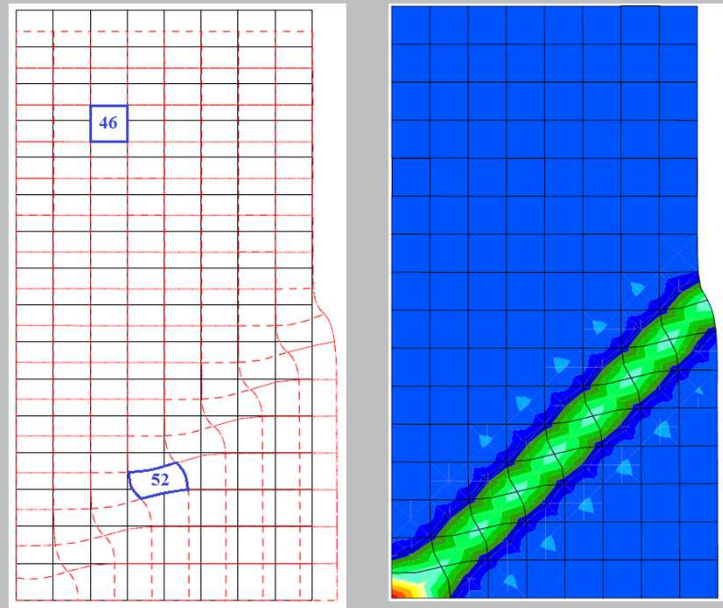
$$\mu = 0.5$$

$$p^* = \frac{f_c}{a \cdot \sigma_0} = 1$$

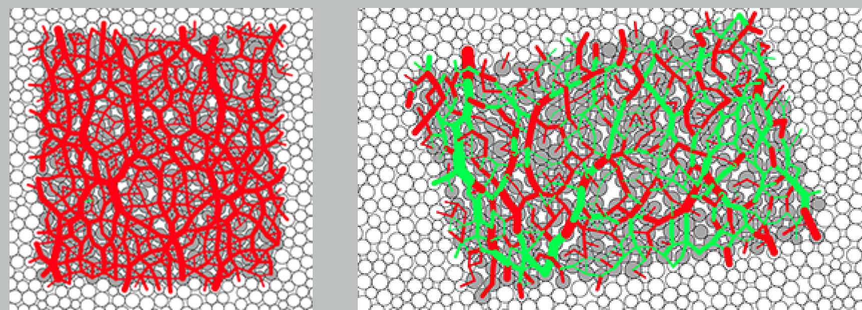
- Macro: discretization by 128 finite elements Q8
- Micro : REV contains 400 grains

Strain Softening and Strain localization : FEM x DEM response





Deformed structure and second invariant of strain tensor



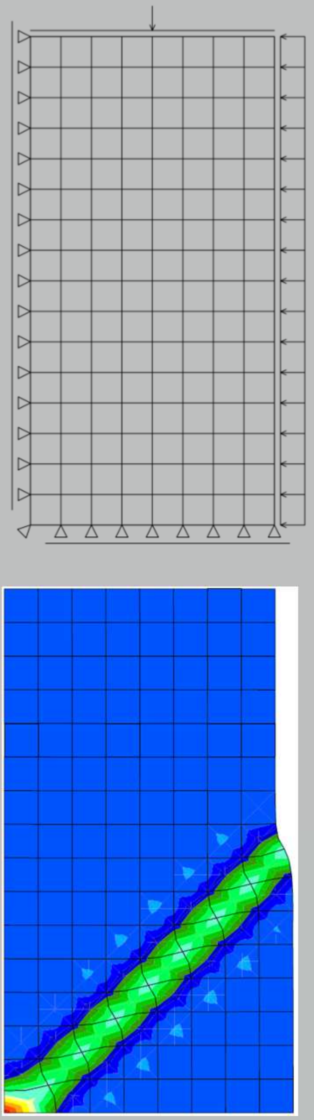
Element 46

Element 52

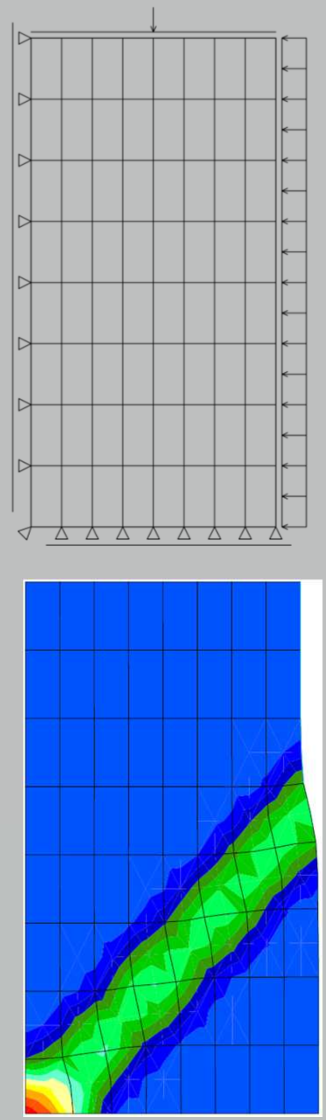
Deformed REV

Multiscale Computations: different meshes

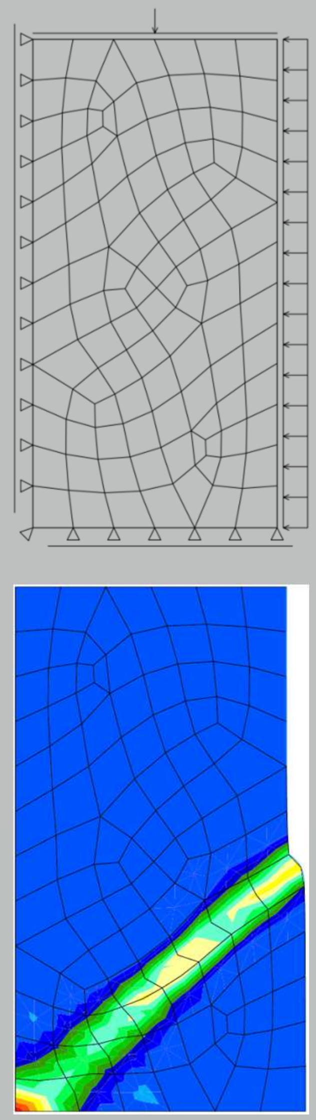
Mesh dependency as usual in FEM : issues and solutions



128 elements



64 elements



106 elements

1. **Triaxial test :**

ideally, should be *homogeneous*, but …

in the lab, observation :

localised deformation

Triaxial test on Hostun sand specimen, JL Colliat, 3SR Grenoble 1986

Second example :

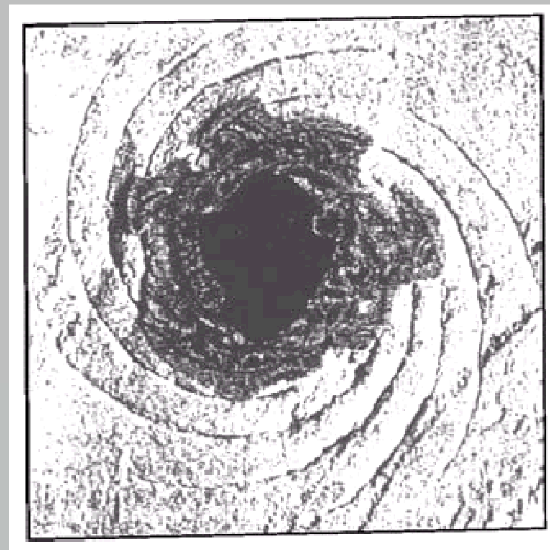
2. **Hollow cylinder under differential pressure**

(analogous to a borehole or a gallery)

heterogeneous by essence

in the field, observation :

localised deformation



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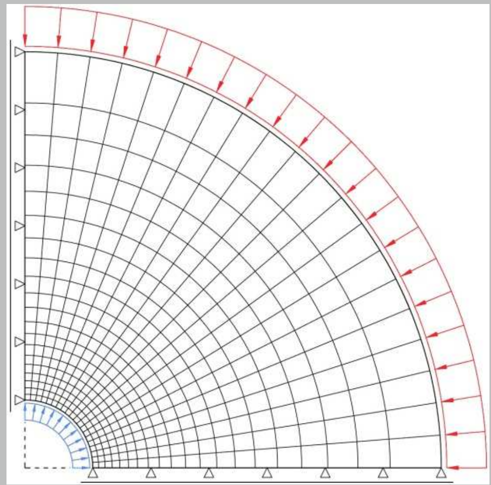
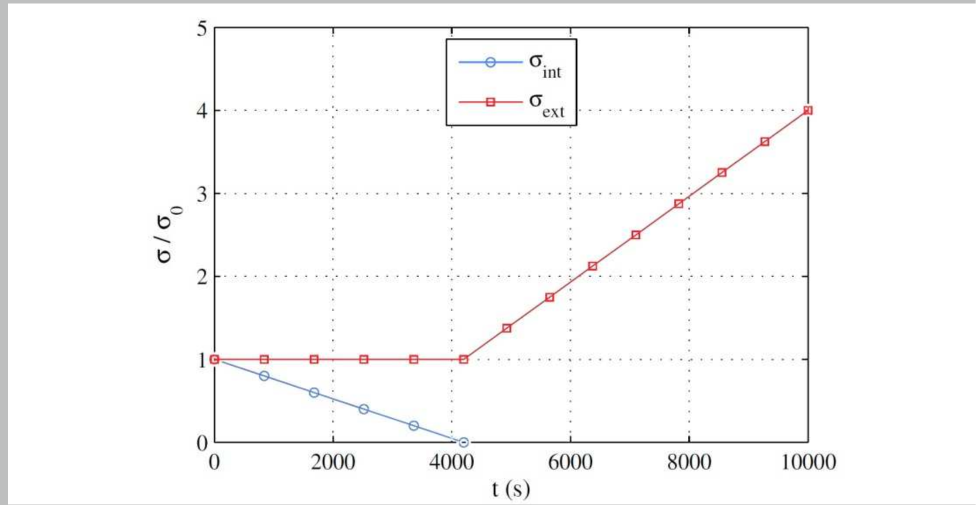
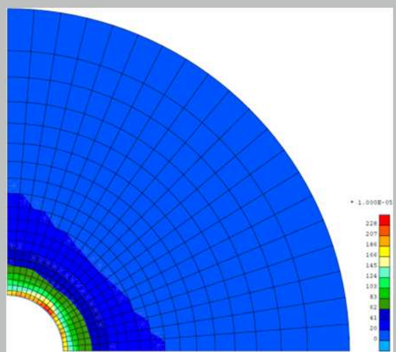
Multiscale Computations: Hollow cylinder (drilling), Strain localization

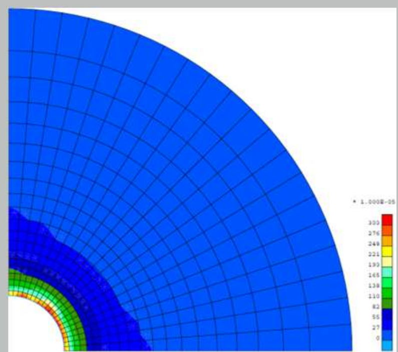




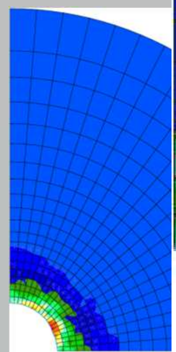
Deformed structure and second invariant of strain tensor



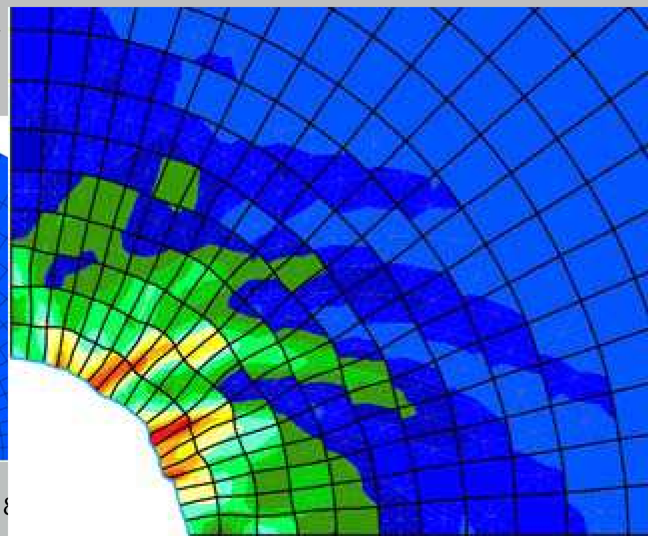
t = 3700
$\varepsilon_{equ\ max}$ = 228. 10^{-5}



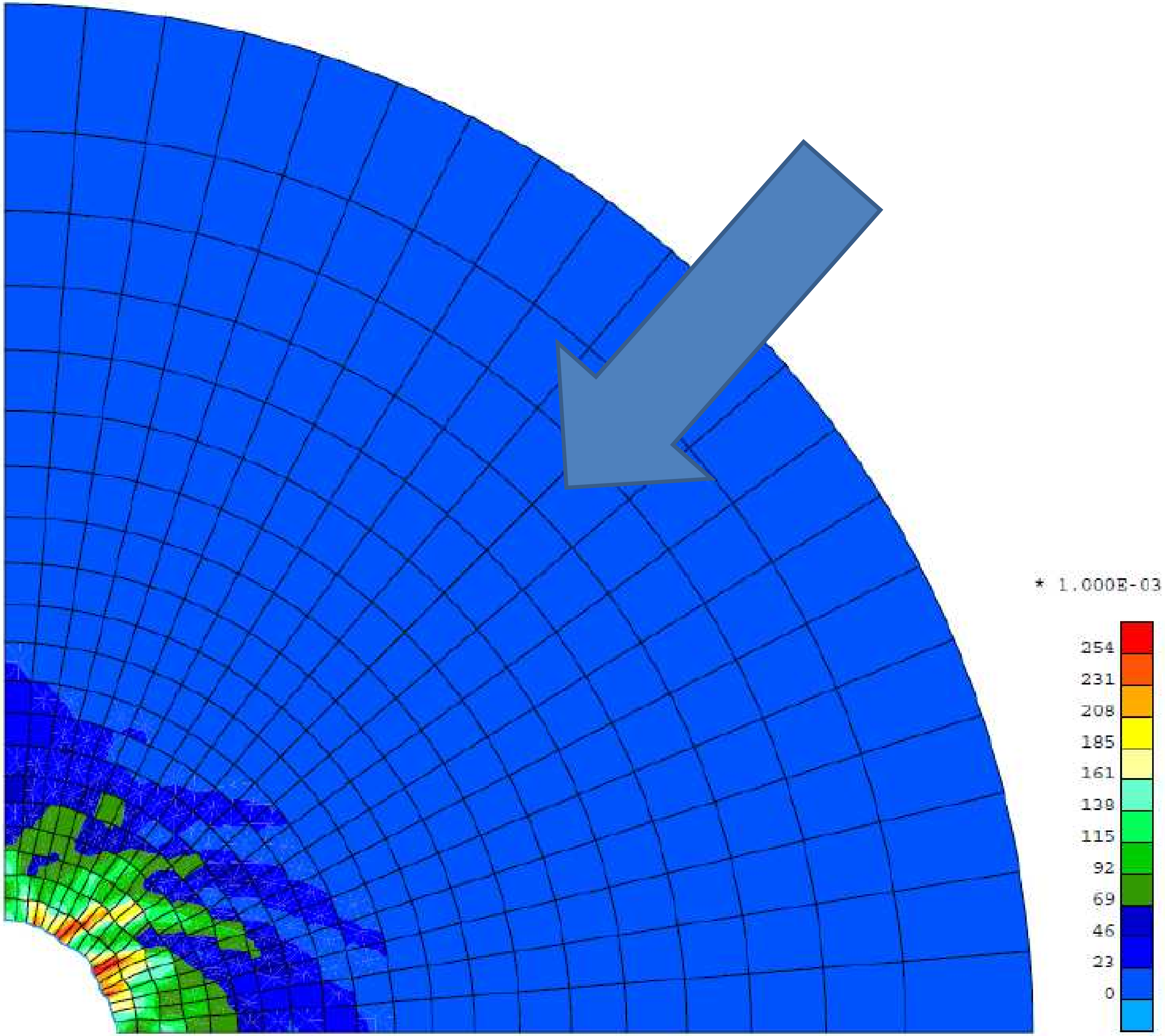
t = 4000
$\varepsilon_{equ\ max}$ = 300. 10^{-5}

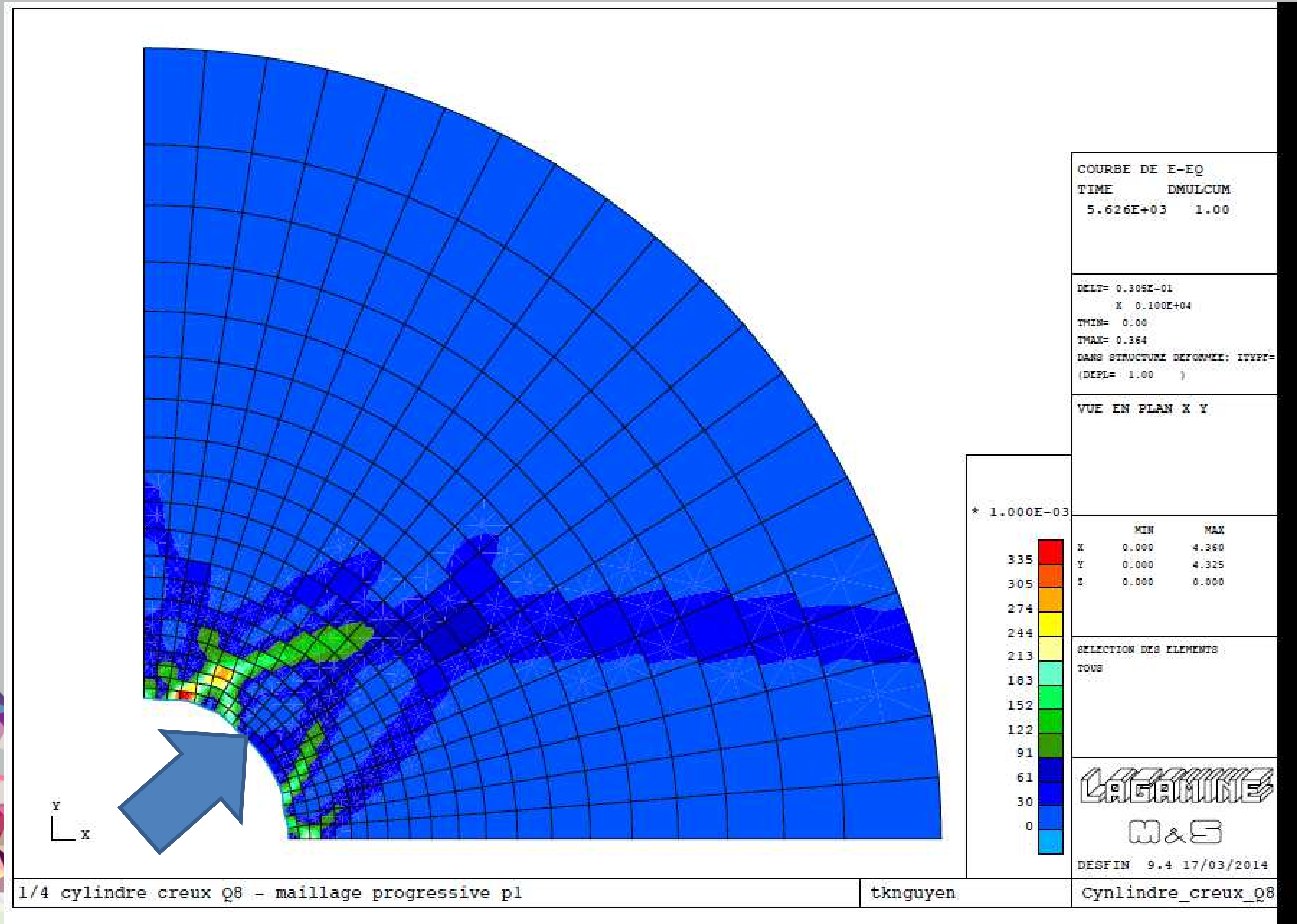


t = 8
$\varepsilon_{equ\ max}$ = 124. 10



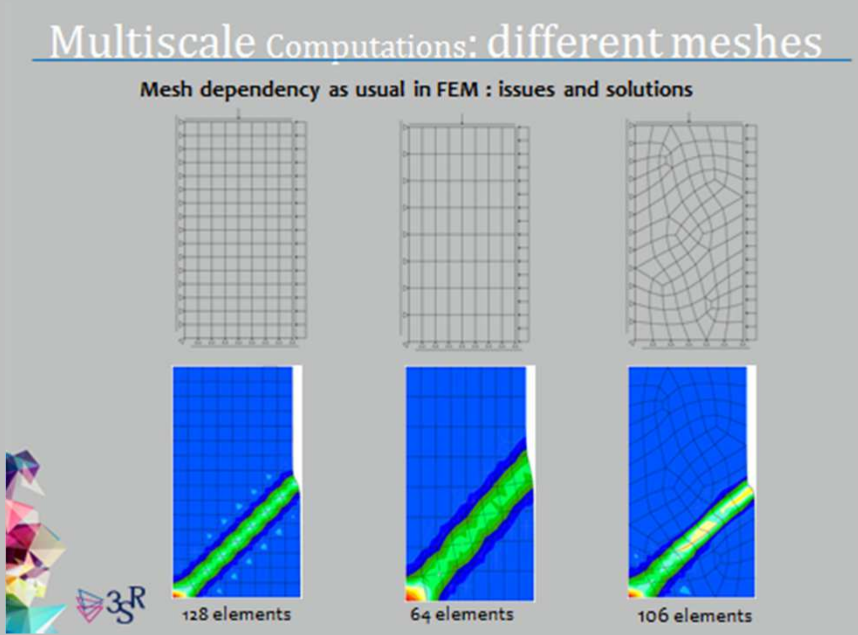
$\varepsilon_{equ\ max}$ = 254. 10

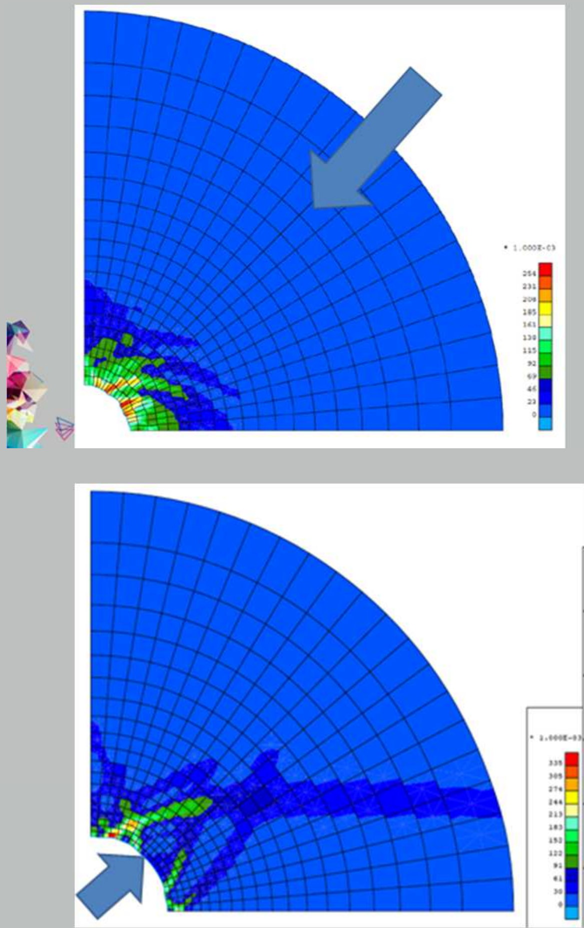

* 1.000E-03
254
231
208
185
161
138
115
92
69
46
23
0


COURBE DE E-EQ
TIME DMULCUM
5.626E+03 1.00
DELT= 0.305E-01
X 0.100E+04
TMIN= 0.00
TMAX= 0.364
DANS STRUCTURE DEFORMEE: ITYPF=
(DEPL= 1.00)
VUE EN PLAN X Y
* 1.000E-03
335
305
274
244
213
183
152
122
91
61
30
0
MIN MAX
X 0.000 4.360
Y 0.000 4.325
Z 0.000 0.000
SELECTION DES ELEMENTS
TOUS
LAGAMINE
M&S
DESFIN 9.4 17/03/2014
Y
X
1/4 cylindre creux Q8 - maillage progressive p1
tknguyen
Cynlindre_creux_Q8

Mesh dependency problem

Solution ?
: regularization of the bvp





Second gradient regularisation
after Chambon R. et al. (1) & Bésuelle P. (2)

- Media with microstructure : enriched kinematics
- macrokinematics
  - u_i is the (macro) displacement field
  - F_{ij} is the macro displacement gradient
    $$F_{ij} = \frac{\partial u_i}{\partial x_j}$$
  - 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 : microkinematics
  - 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:
    $$h_{ijk} = \frac{\partial f_{ij}}{\partial x_k}$$: Local second gradient
- The internal virtual work

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

1 – Chambon R., Caillerie D., Matsushima T. (2001) **Int. Journal of Solids and Stuctures** vol.38 No 46-47, pp. 8503-27
2 –Bésuelle et al. (2006) **Journal Of Mechanics Of Materials And Structures** Vol. 1, No. 7, pp 1115-34

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- enrichment : microkinematics
  - 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

Additional kinematical constraint : $f_{ij} = F_{ij}$

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

1 – Chambon R., Caillerie D., Matsushima T. (2001) **Int. Journal of Solids and Stuctures v**ol.38 No 46-47, pp. 8503-27

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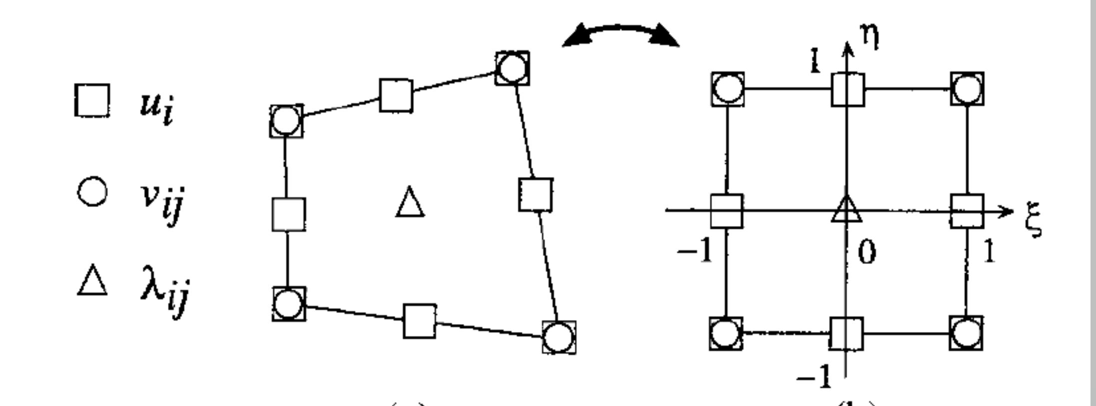
Second gradient regularisation (cont'd)

after Chambon R. et al. (1) & Bésuelle P. (2)

- FEM : introducing Lagrange multipliers to enforce the condition $f_{ij} = F_{ij}$:

$$\int_{\Omega^t} (\sigma_{ij}^t \frac{\partial u_i^\star}{\partial x_j^t} + \chi_{ijk}^t \frac{\partial v_{ij}^\star}{\partial x_k^t}) d\Omega^t - \int_{\Omega^t} \lambda_{ij}^t (\frac{\partial u_i^\star}{\partial x_j^t} - v_{ij}^\star) d\Omega^t - \bar{P}_e^\star = 0$$



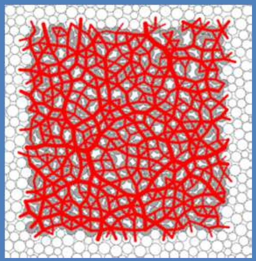
(a) (b)

1 – Chambon R., Caillerie D., Matsushima T. (2001) **Int. Journal of Solids and Stuctures** vol.38 No 46-47, pp. 8503-27
2 –Bésuelle et al. (2006) **Journal Of Mechanics Of Materials And Structures** Vol. 1, No. 7, pp 1115-34

Second gradient regularisation (cont'd)

- A 2nd gradient model for FEM-DEM double scale analysis

- **Constitutive equations :**
  - Classical part : LHN_DEM

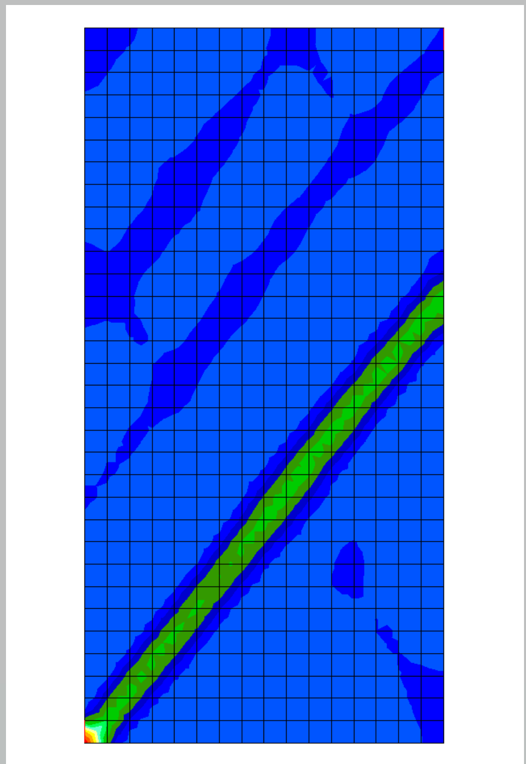


  - 2nd gradient part : only 1 parameter D

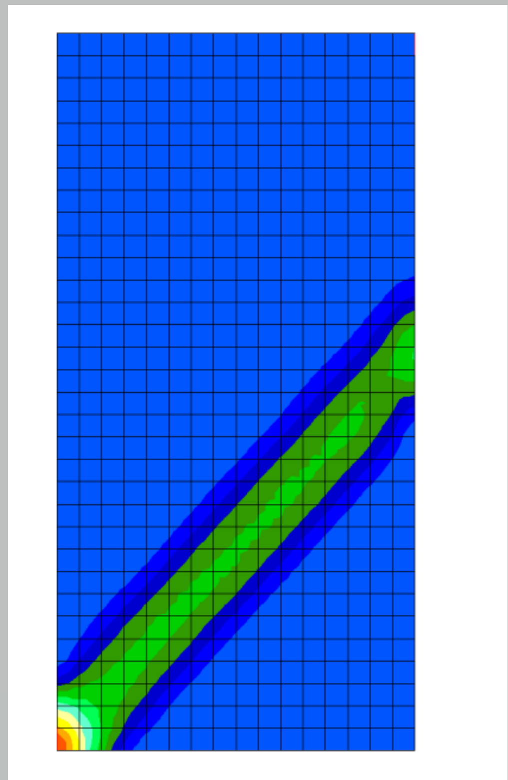
$$
\begin{bmatrix} \overset{\nabla}{\chi}_{111} \\ \overset{\nabla}{\chi}_{112} \\ \overset{\nabla}{\chi}_{121} \\ \overset{\nabla}{\chi}_{122} \\ \overset{\nabla}{\chi}_{211} \\ \overset{\nabla}{\chi}_{212} \\ \overset{\nabla}{\chi}_{221} \\ \overset{\nabla}{\chi}_{222} \end{bmatrix}
=
\begin{bmatrix}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

Restoring mesh independency with 2nd gradient

- No 2nd gradient
- With 2nd gradient



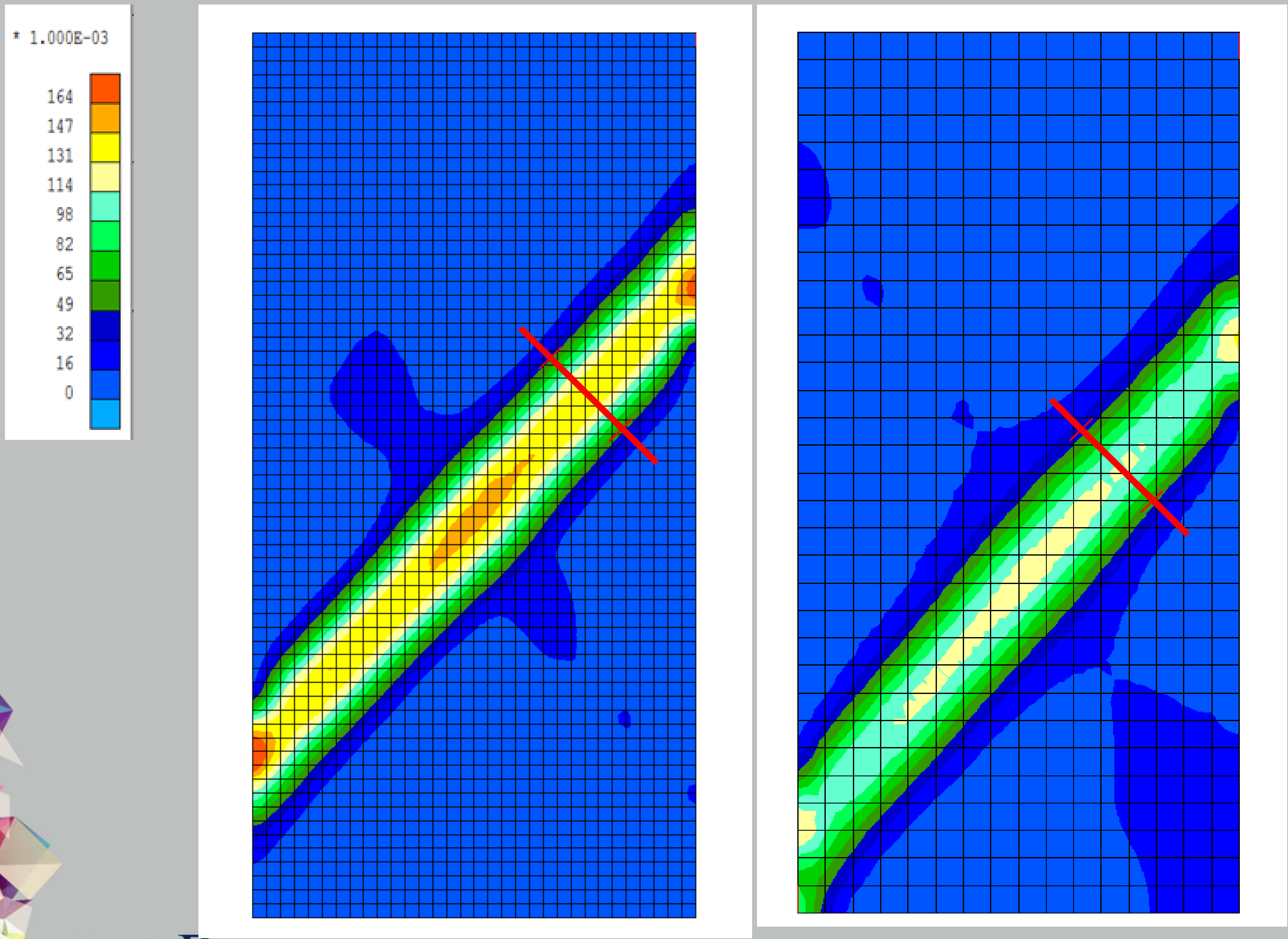
512 FE x 400 DE



512 FE x 400 DE

Second Gradient D=0,64E-2

Axial strain = 2. 10-2

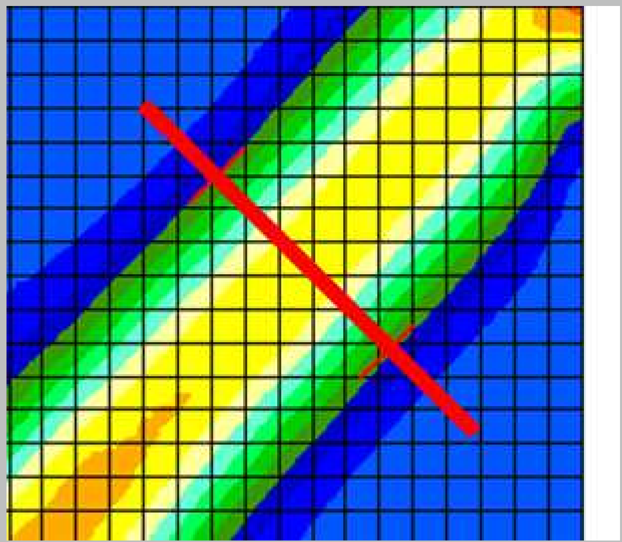


2048FEMx400DEM

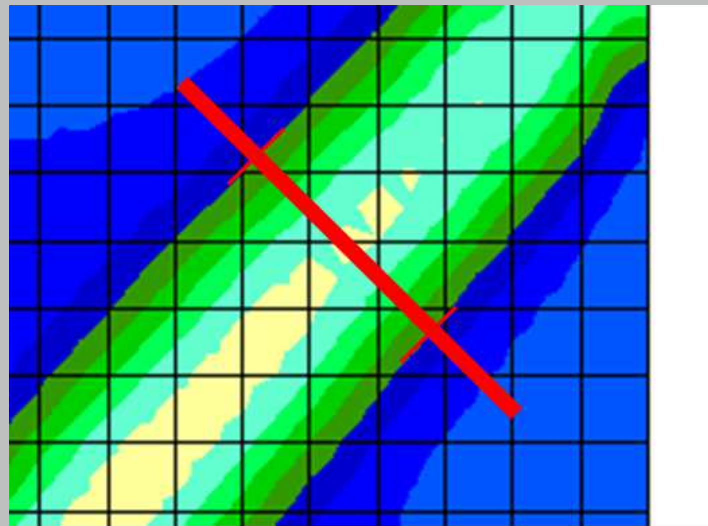
512FEMx400DEM

Restoring mesh independency with 2nd gradient

Second Gradient D=0,64E-2



2048 FE x 400 DE



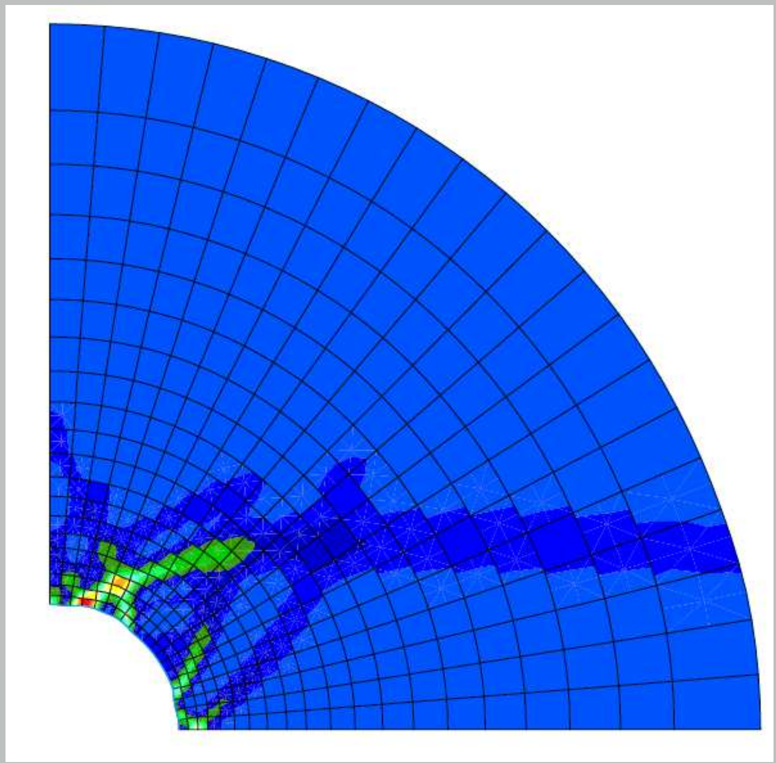
512 FE x 400 DE

2048FEMx400DEM

512FEMx400DEM

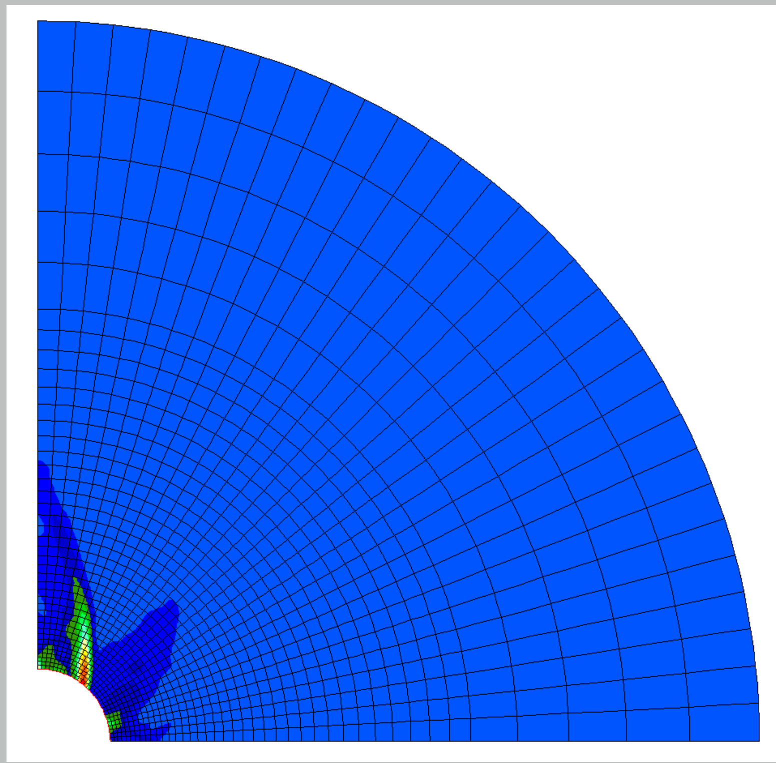
Restoring mesh independency with 2nd gradient

- No 2nd gradient



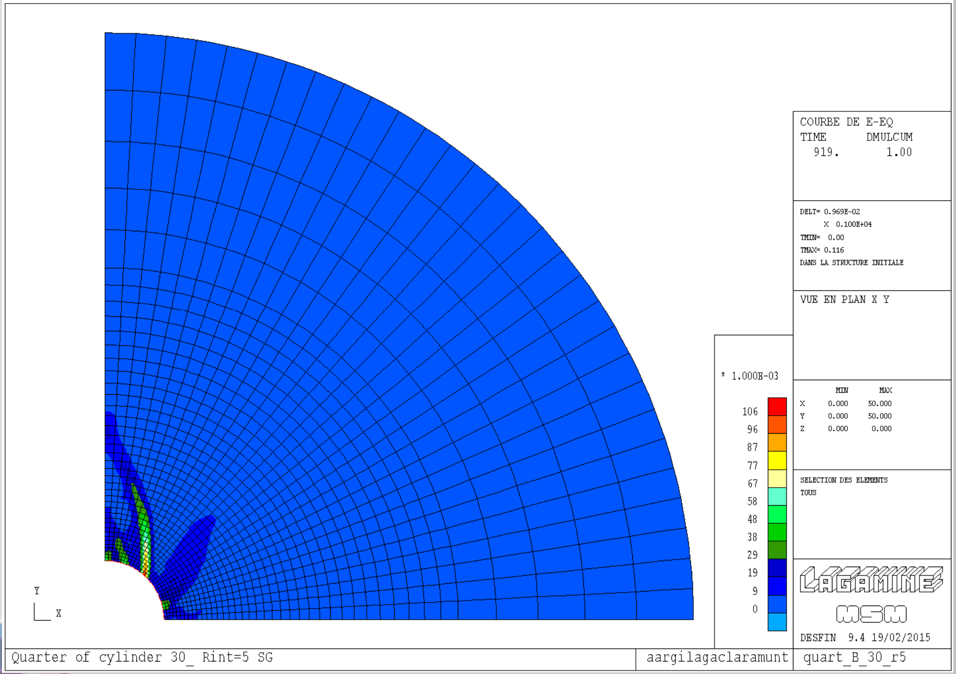
400 FE x 400 DE

- With 2nd gradient

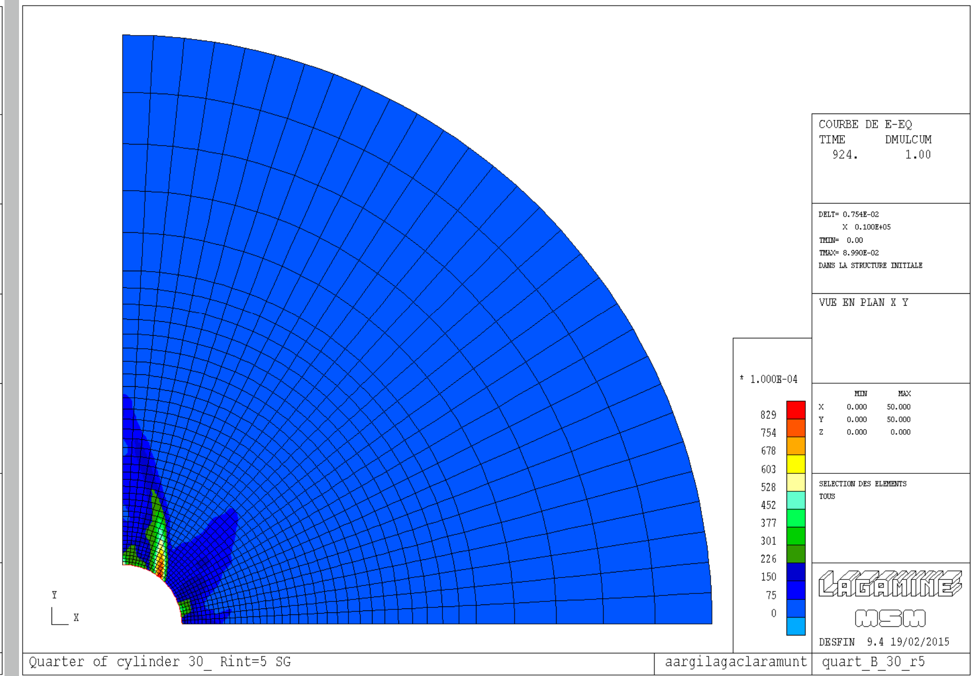


1230 FE x 400 DE

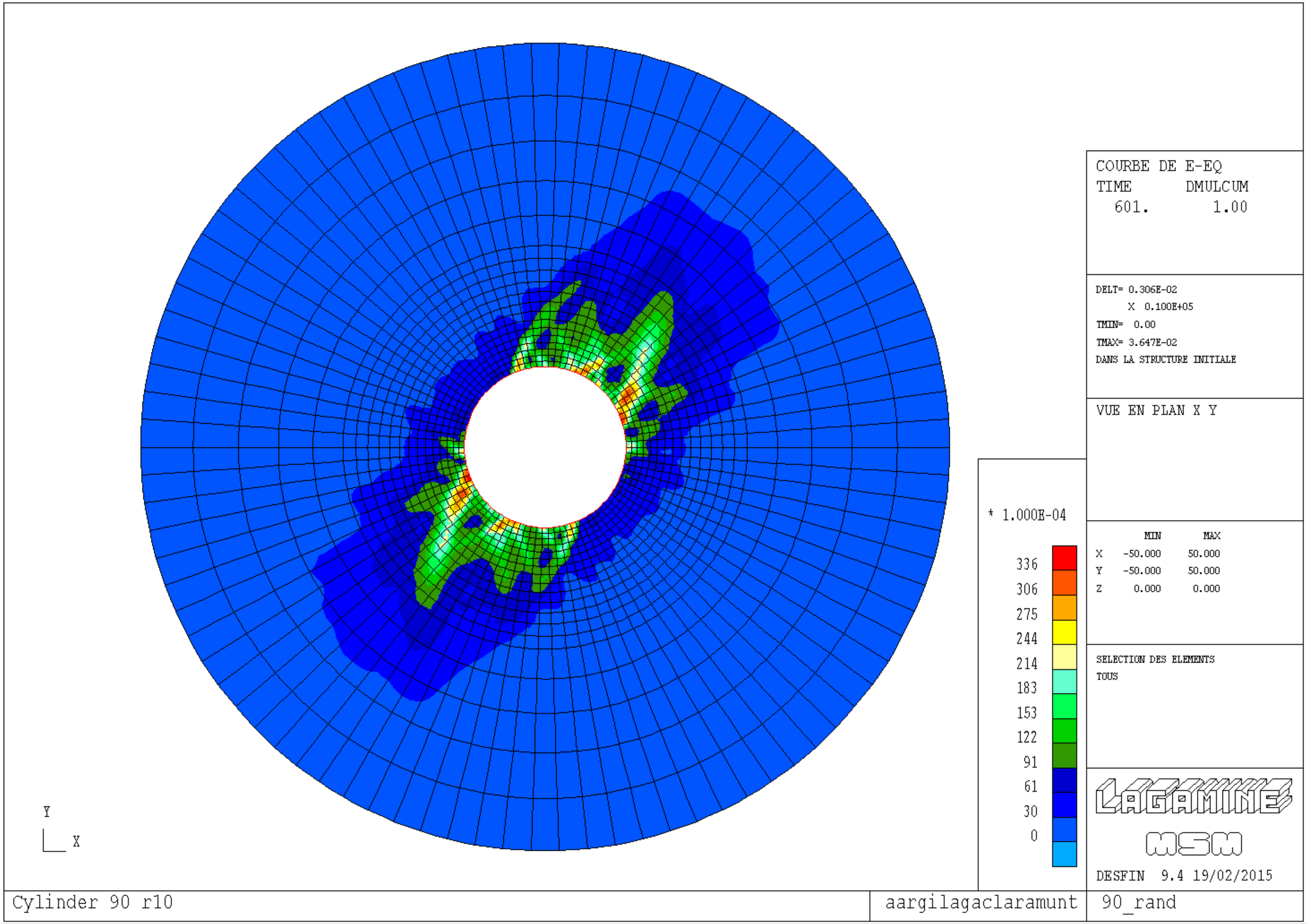
1290FEMx400DEM Loading: increase internal pressure



Second Gradient D=5,00E-2



Second Gradient D=1,00E-1 (x2)



1980FEMx400DEM Second Gradient D=1,25E-2 Loading: increase internal pressure

Conclusions & Perspectives

CONCLUSIONS

- We have presented a Two-scale numerical approach for granular materials: combining FEM (at macro scale) and DEM (at micro scale).
    - Illustration by two examples of BVP :
        - a biaxial compression test and
        - a hollow cylinder (analogy of underground excavations and drilling)
    - Strain localization was observed in both cases.
    - Mesh dependency confirmed.
- 2nd gradient regularization allows to restore mesh *independency*
    - Mesh independency is restored
    - Parallelisation of the code (element loop) using OpenMP has showed to be very effective

PERSPECTIVES

-3D approach

-HPC high performance computing (calcul intensif) :

OpenMP & MPI parallel computing schemes

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A FE^2 model for hydro-mechanical coupling in a brittle material

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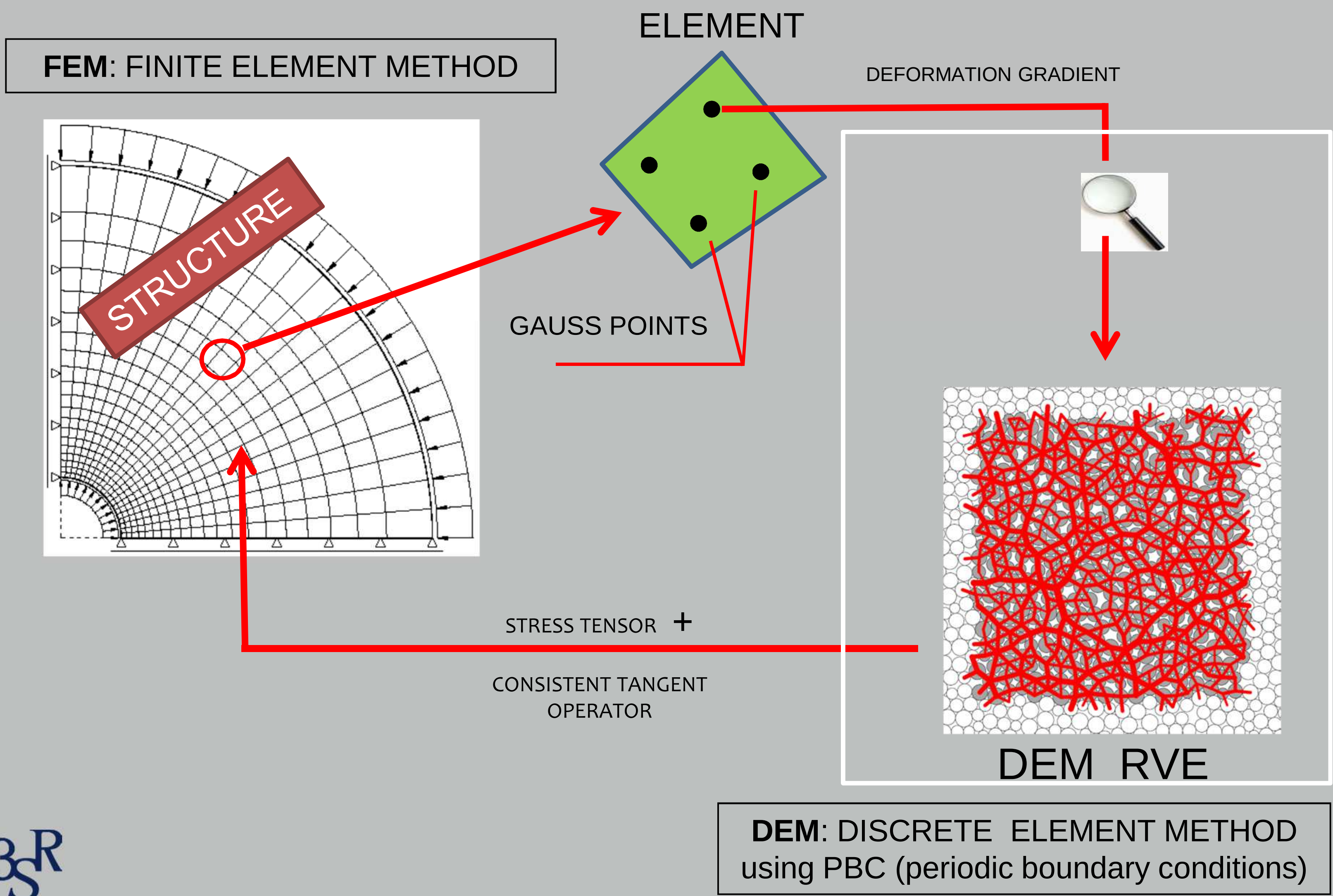
[2] University of Liège, Belgium

[3] Andra, France

Tsukuba – March 12th 2015

Principle FEM x DEM

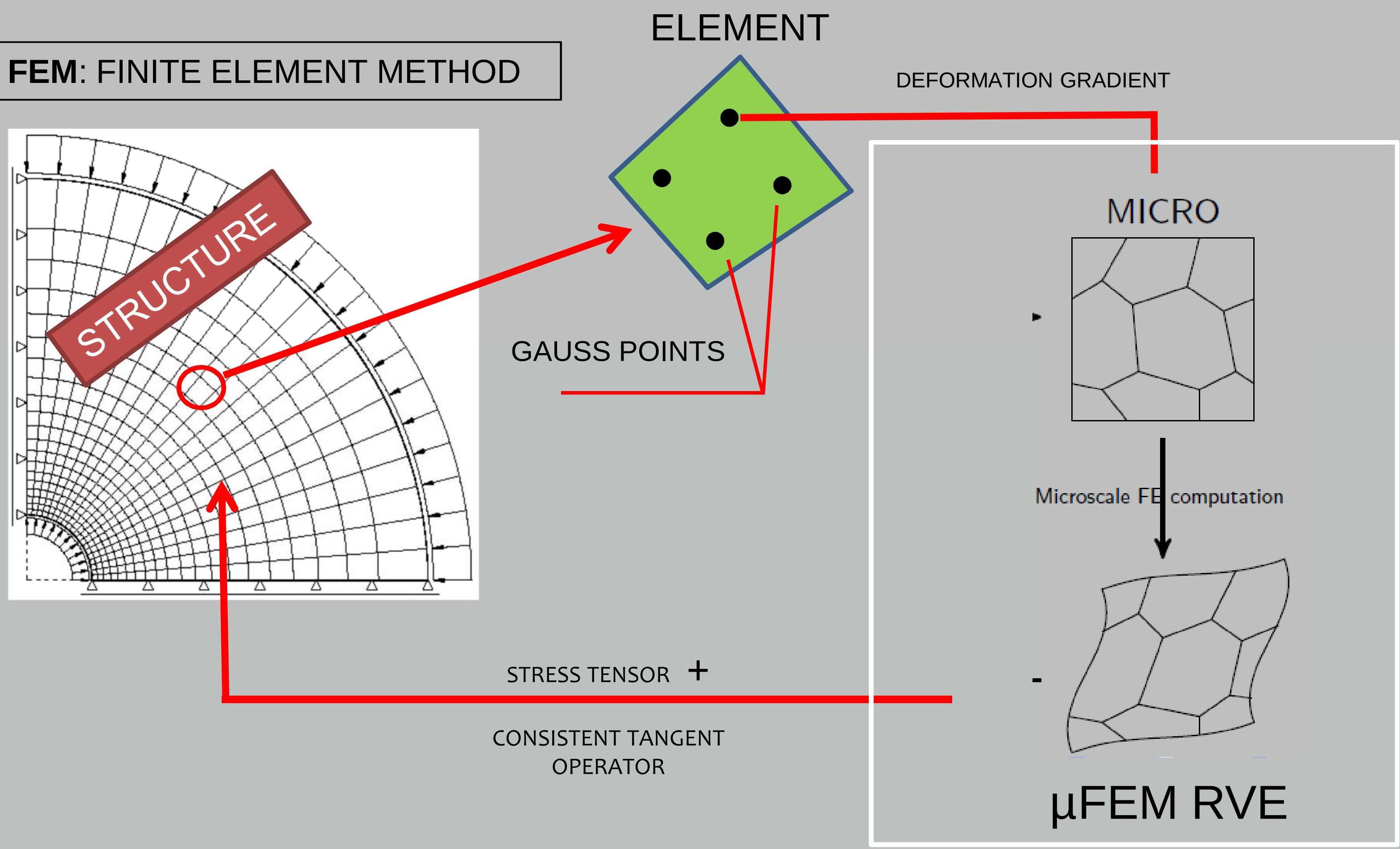
A two-scale numerical homogenization approach by FEM - DEM



Principle FEM^2

A two-scale numerical homogenization approach by FEM - DEM

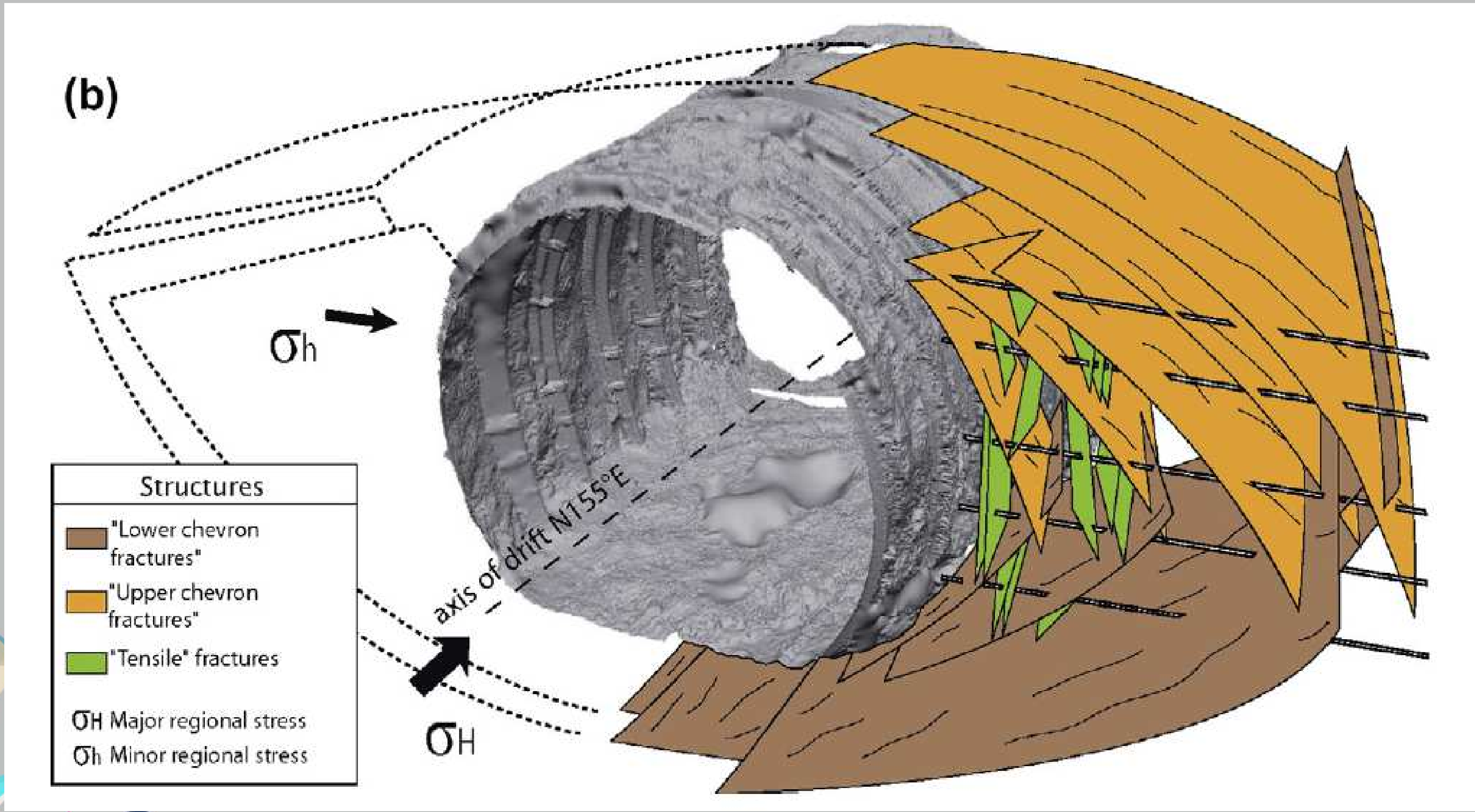
FEM: FINITE ELEMENT METHOD



µFEM: FINITE ELEMENT METHOD using PBC (periodic boundary conditions)

La problématique de l'EDZ
autour des galeries dans les roches argileuses

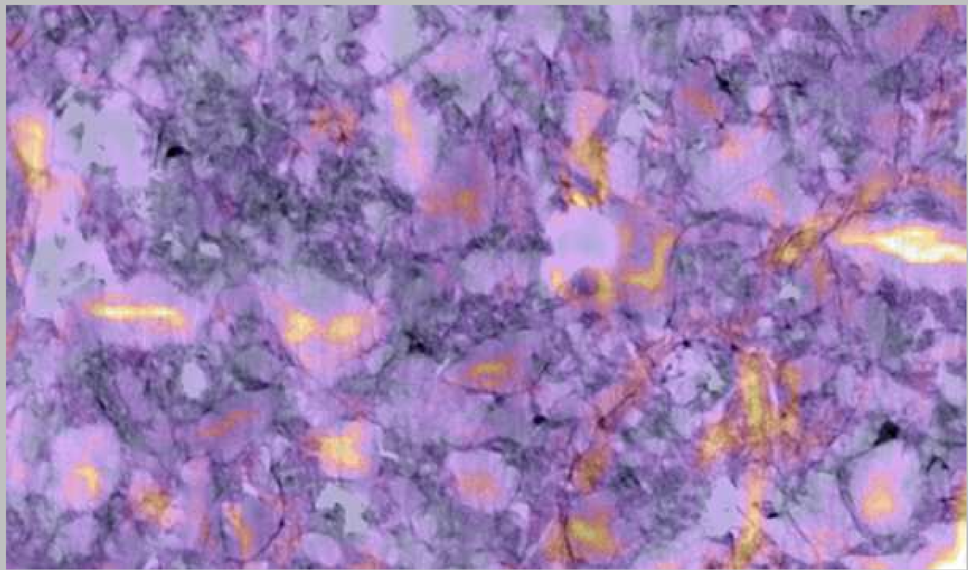
contexte ouvrages de stockage de déchets nucléaires
(données ANDRA)



Motivations

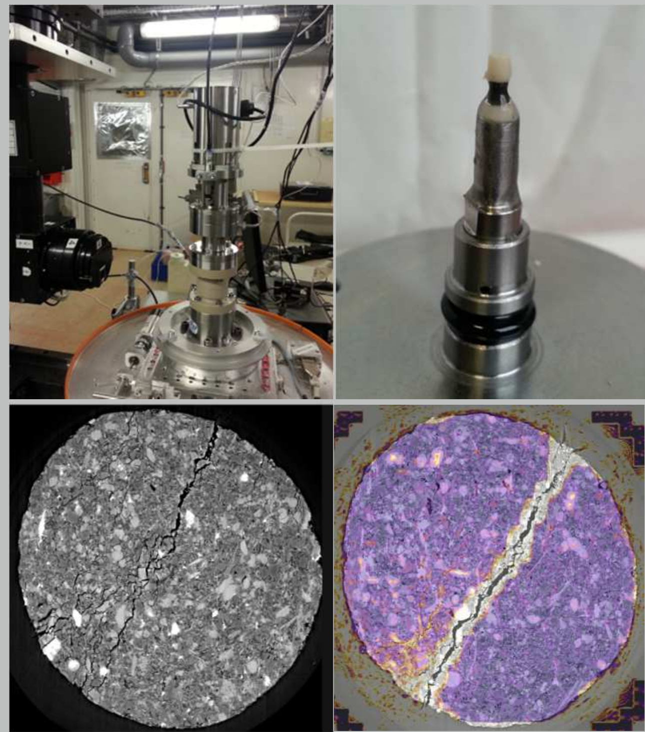
Microstructure of the clay-rock

▸ Micromechanisms of deformation



10µm

Overlapping between X-ray ηano-CT and incremental 2nd strain invariant field (DIC)



100µm

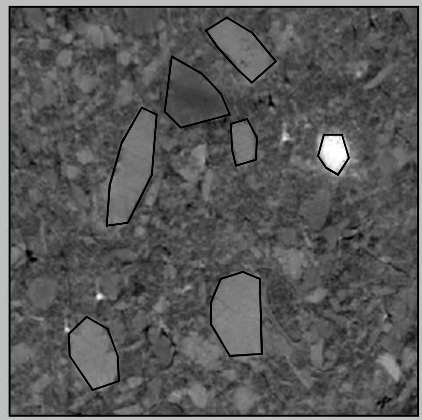
In situ triaxial loading test at ESRF (ID19)

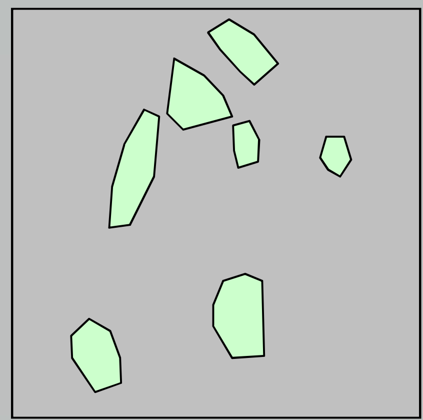
X-ray nanotomography + volume DIC

Bésuelle *et al.*, 2013

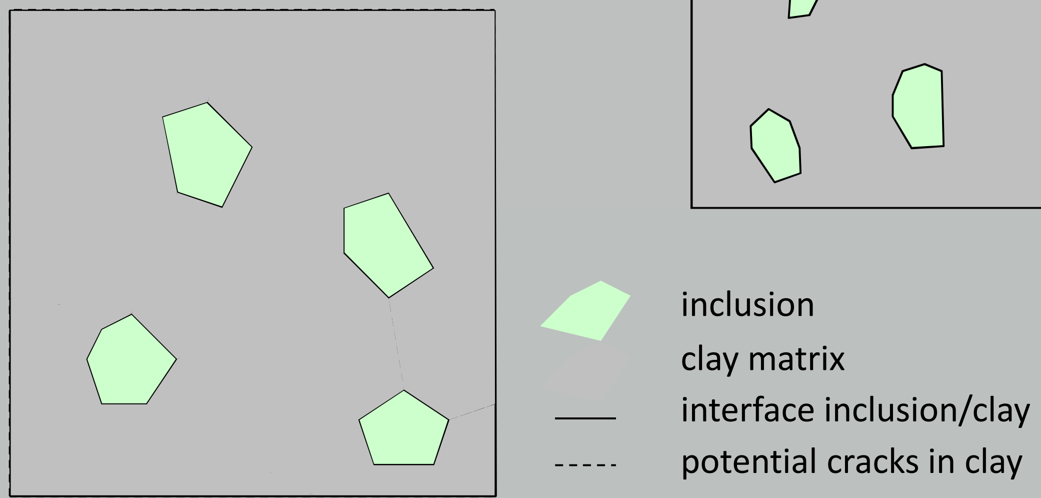
Motivations

Microstructure of the clay-rock



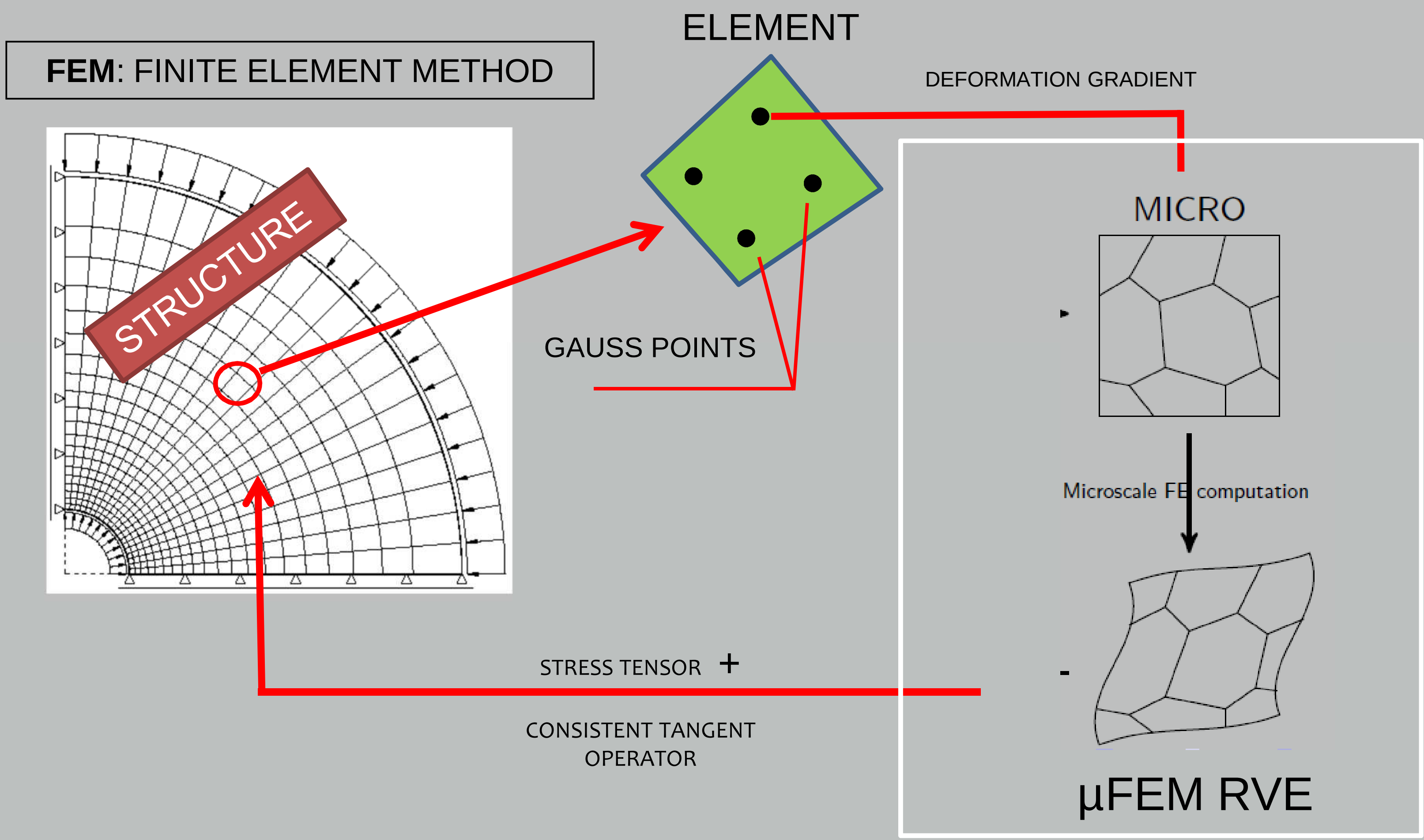


Representative elementary volume (REV)



Principle FEM^2

A two-scale numerical homogenization approach by FEM - DEM



μFEM: FINITE ELEMENT METHOD using PBC (periodic boundary conditions)

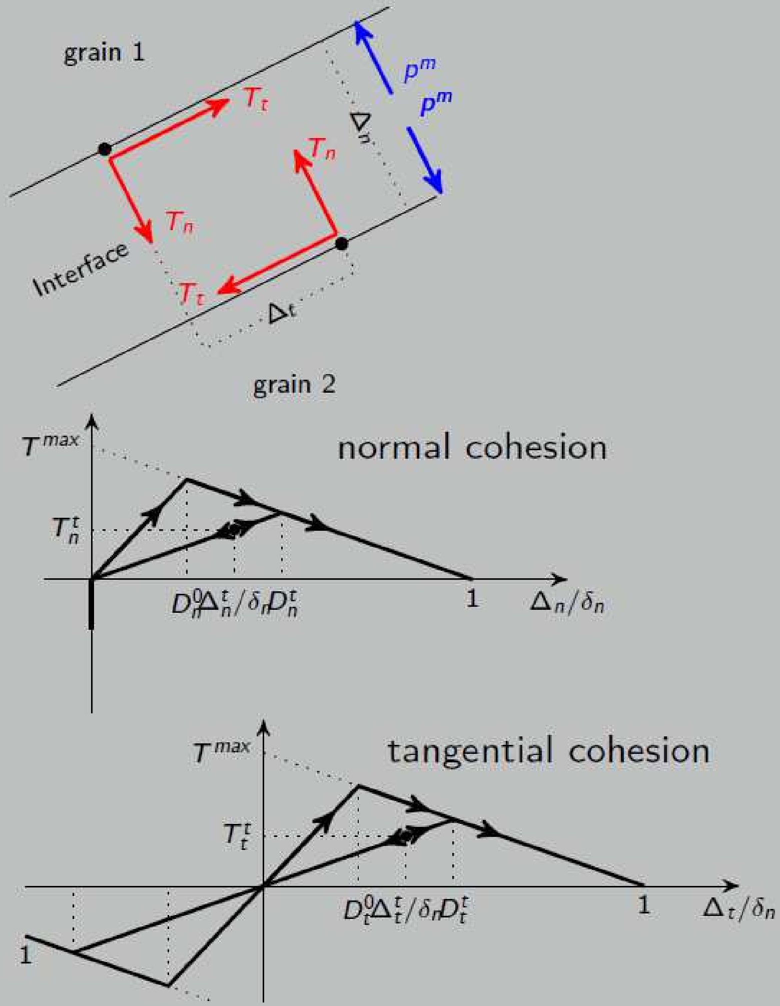
MICROSCALE PROBLEM

Micro REV: mechanical model (constitutive laws)

- Grains :
  - Linear elastic solids

$$\sigma_{ij} = \delta_{ij}\lambda tr(\varepsilon) + 2\mu\varepsilon_{ij}$$

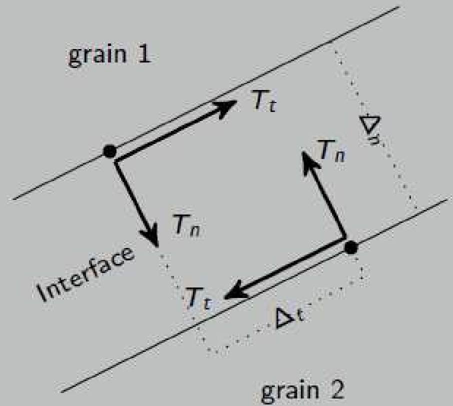
- Interfaces:
  - Damage laws



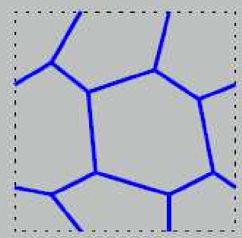
Microscale problem

Micro REV: hydraulic model

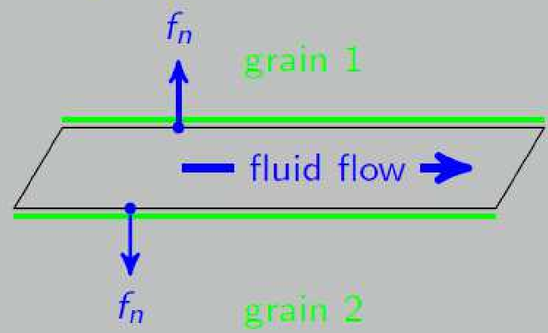
- Cohesive interfaces (coupling M → H)
  - Interface opening defines channel hydraulic conductivity ($\kappa \propto \Delta h^3$)



- Flow assumptions
  - Laminar flow between smooth parallel platens
  - Network of 1D channels between grains
  - System of equations for flow in an element



- Fluid forces (coupling H → M)
  - Fluid pressure acting normally on solids boundaries



DOUBLE SCALE COMPUTATIONS

Strain localization

- Strain localization and fluid flow

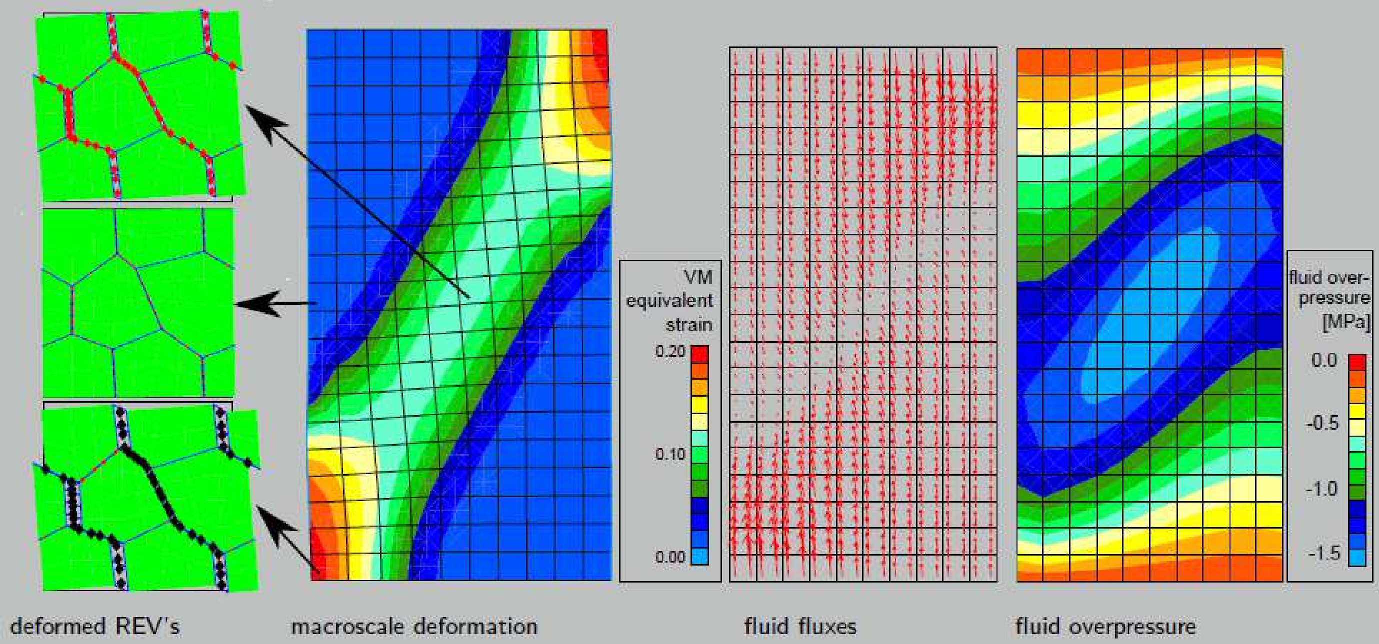
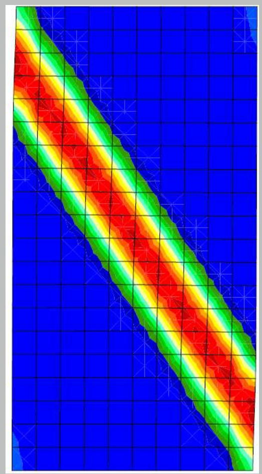


Figure : Hydromechanical state at 1.5% axial strain

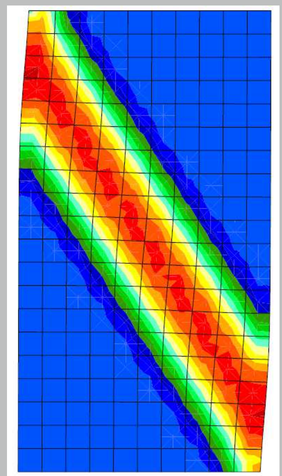
MACRO FIELD EQUATIONS

Second gradient continuum with Hydro-Mechanical coupling

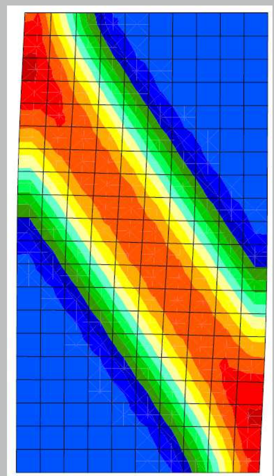
The band thickness depends on constitutive parameters of the model (no mesh size dependence, if the mesh is sufficiently fine / internal length)



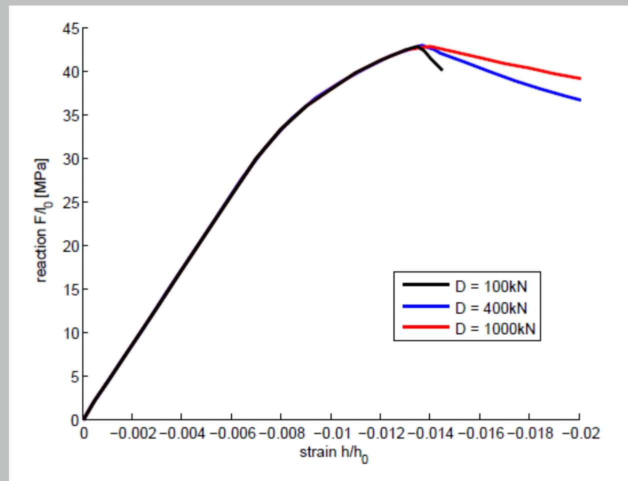
D = 1.0^{E+5}N



D = 4.0^{E+5}N



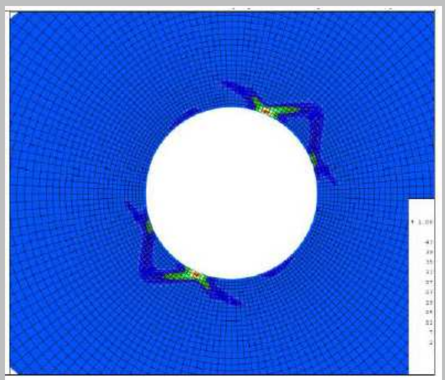
D = 1.0^{E+6}N

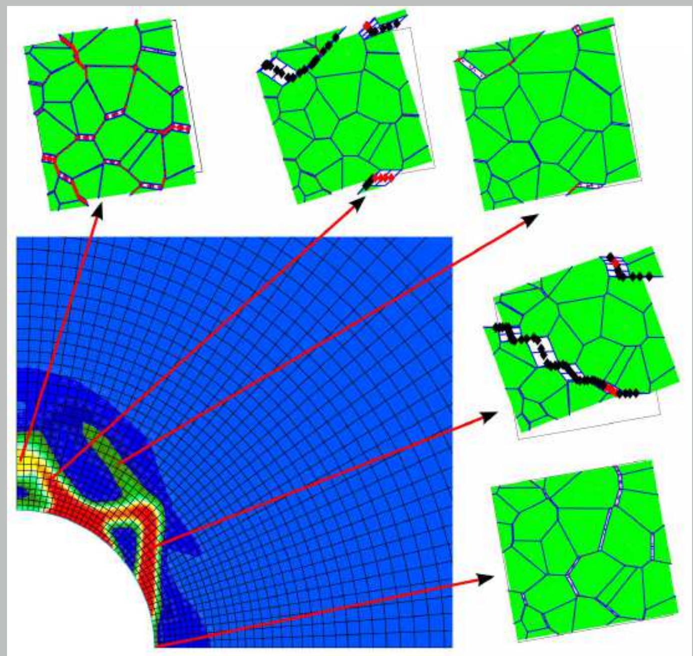


Double scale computations

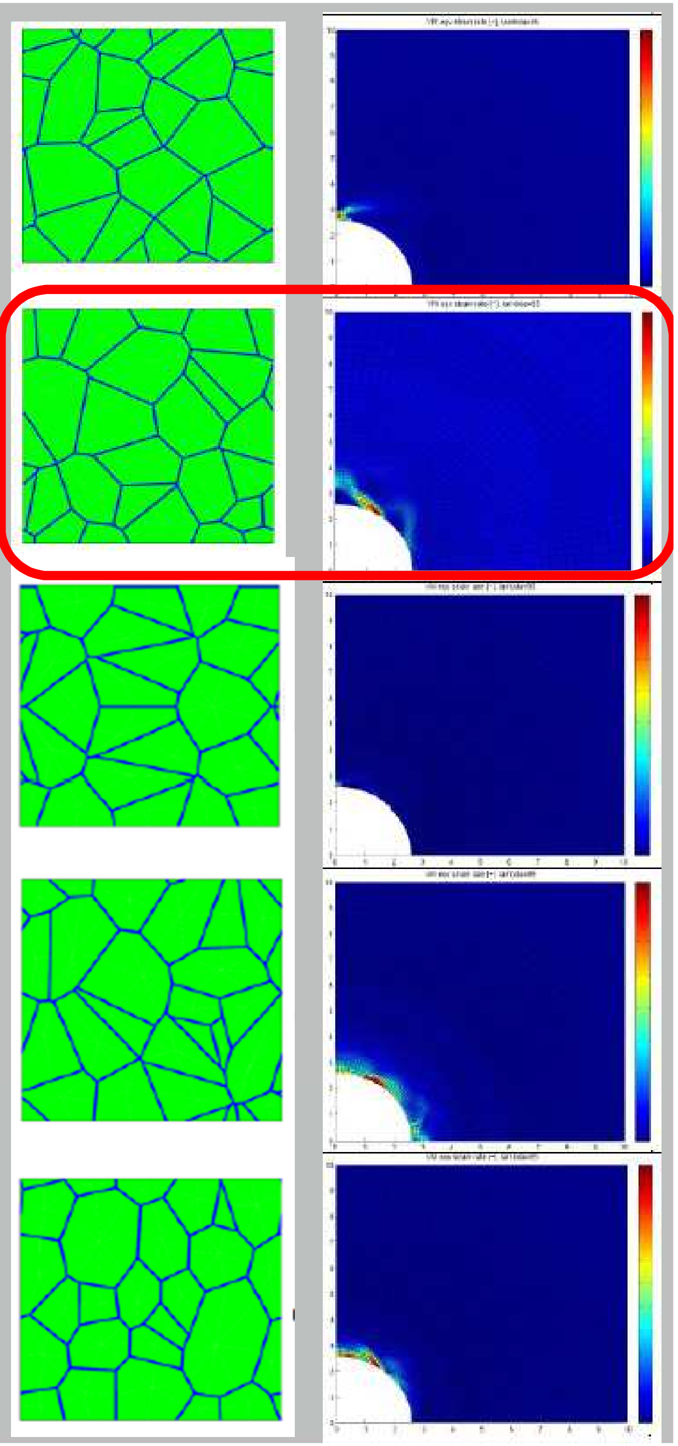
Strain localization and anisotropy

- Failure during a gallery excavation: depressurization of the internal pressure, constant external pressure
- 1600 elements
- Constitutive parameters calibrated to fit experimental curves
- Strain localization pattern influenced by the anisotropy of the model





dry material



DOUBLE SCALE COMPUTATIONS

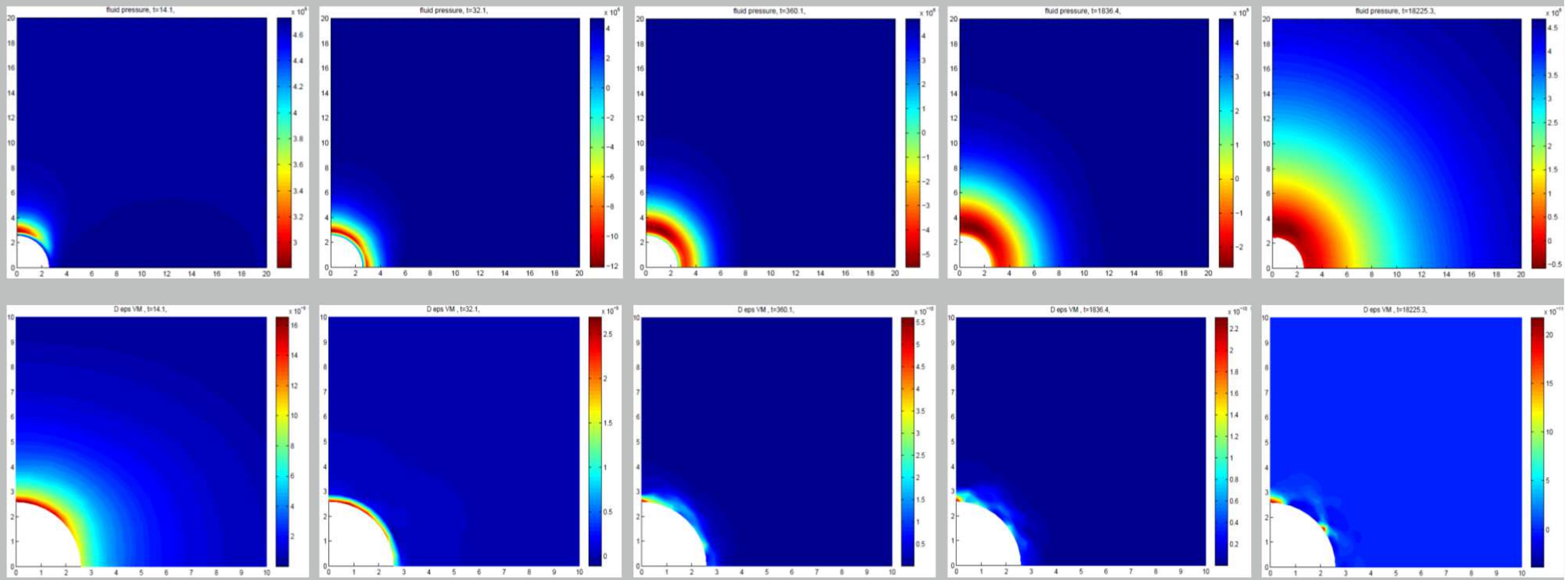
Strain localization, anisotropy and fluid flow

wet material

14 days | 1 month | 1 year | 5 years | 50 years

pore pressure

deviatoric strain rate



Conclusions and perspectives

Conclusions

- The FE^2 approach with local second gradient framework is demonstrated to be suitable for the modelling of hydromechanical coupling
- The FE^2 model has been introduced in the FE code *Lagamine* (Liège)
- Complexity of the macroscale response can be taken into account, based on realistic microstructures: anistropy, damage, full loading history, strain localization, etc…

Perpectives

- The micromechanical model can be extended: double porosity, non-elastic grains, more general interface law, time dependence, etc…
- Model calibration: macro and micro experimental characterization
- Reduction of computation time (numerical parallelization, etc…)