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From discrete to continuum approach of Boundary Value Problems in Geomechanics : FEMxDEM integrated approach

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Modern Trends in Geomechanics 2016– Assisi – 16-18 May 2016

Outline

1. Introduction : principle
2. Micro-scale (DEM) Model
3. Multi-scale Coupling Method
4. FEM-DEM simulations
5. 2^{nd} gradient : motivation, methods and results
6. Cpu cost issue : parallelization solution
7. Conclusions & Perspectives

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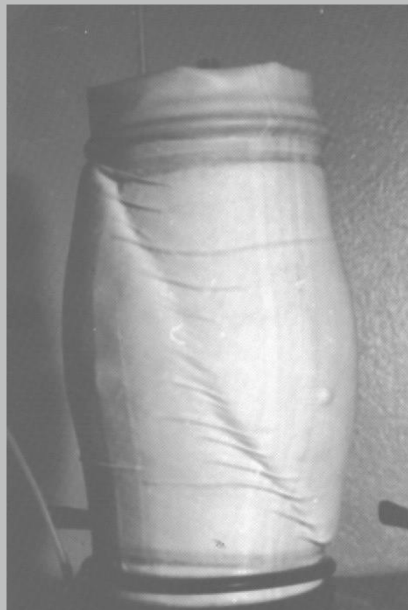
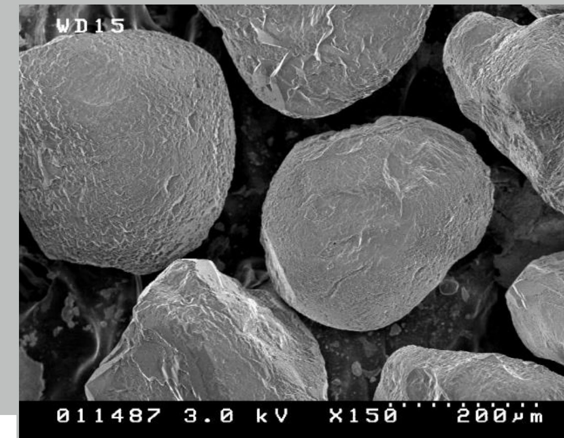
Introduction : bridging scales in Geomechanics :

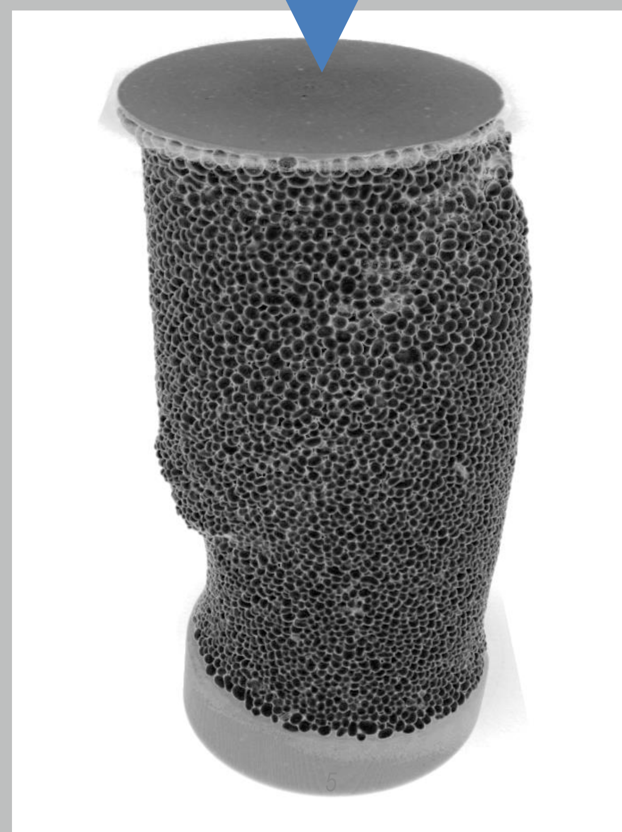


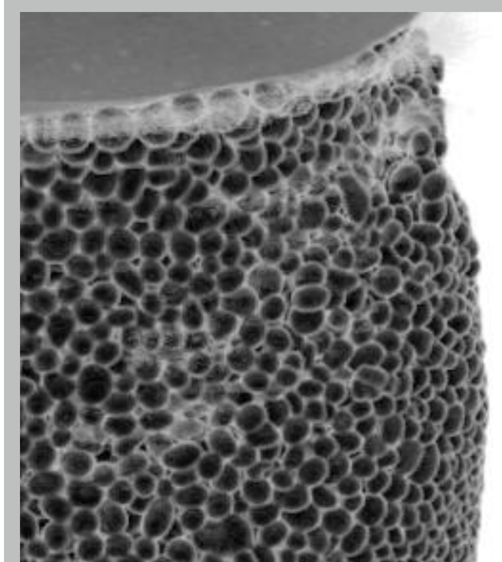
in experiments …

?

High resolution
XR tomography (> 2000)







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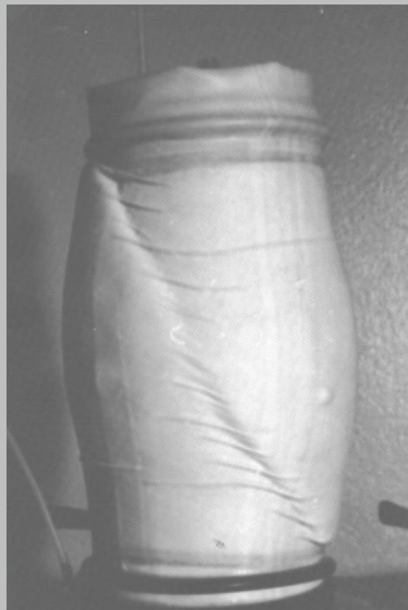
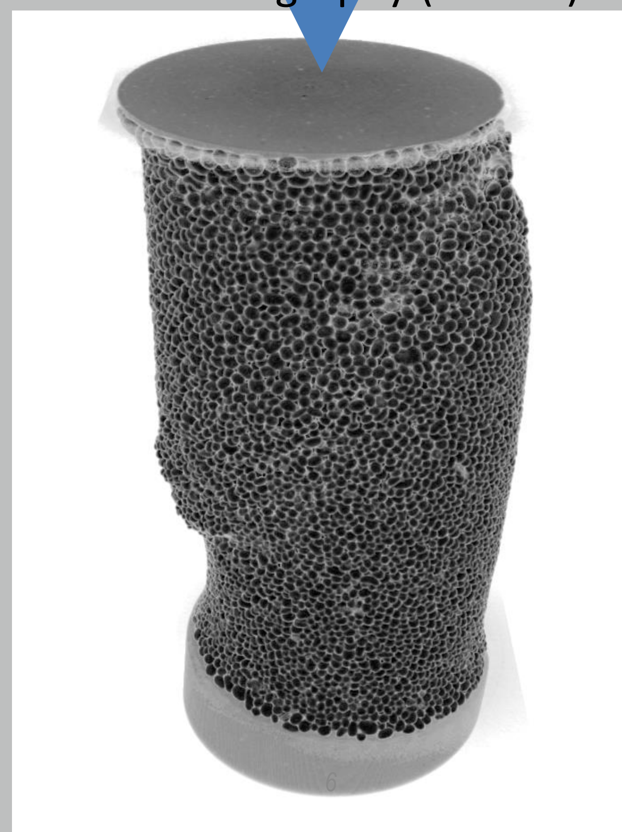
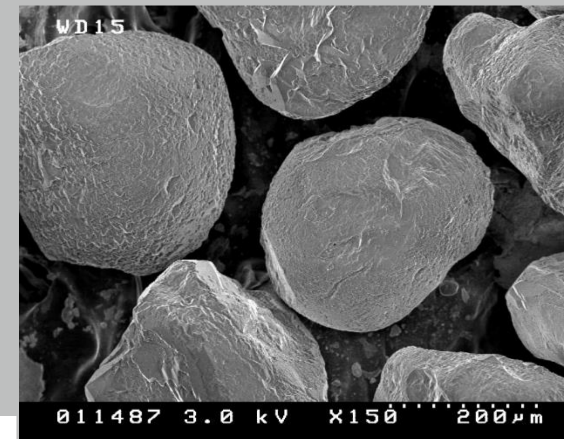


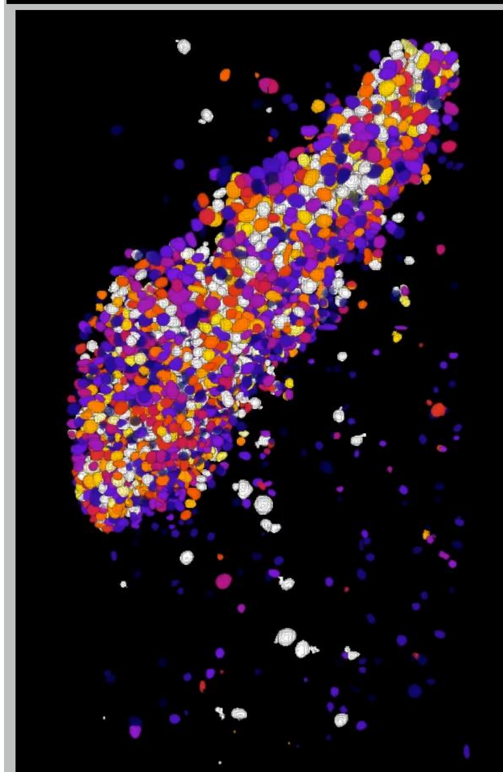
in experiments …

?

High resolution
XR tomography (> 2008)







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

bridging scales in Geomechanics : **modelling**

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

Continuum : FEM	Particles : DEM
☺ well suited to Real scale problem ☹ simply *disregard* the discrete nature of granular media : instead, accounts for the observed consequences of this *discrete nature* through *formal* constitutive equations > always lacking generality, because the general behaviour is too complex	☺ Reproduces « naturally » the complex behaviour of grains assembly : cyclic response, anisotropy, strain path dependency, strain softening ☹ 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

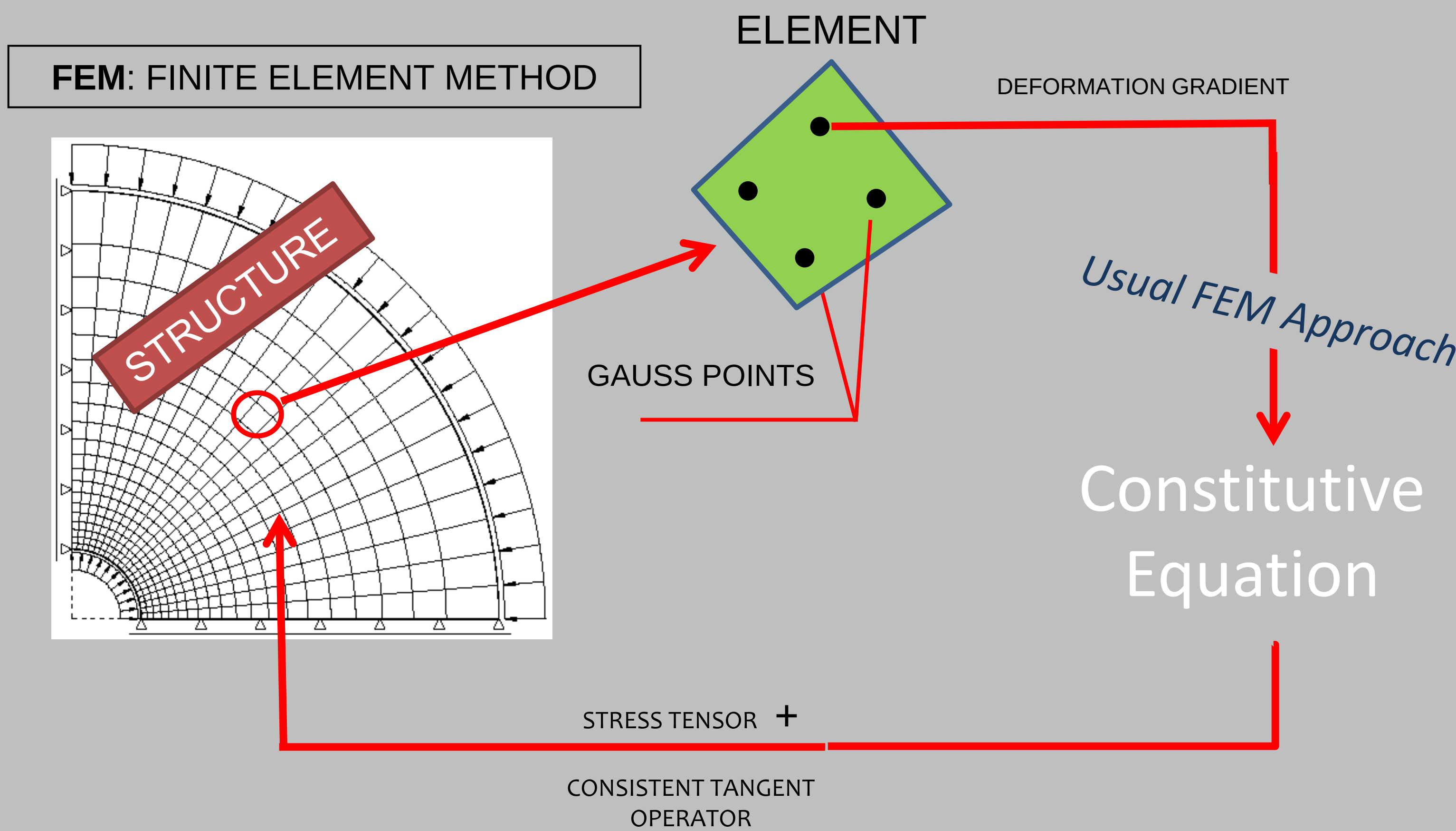
A rather recent trend in geomaterials, a few teams in the world :

(not all the papers of each team,
may be not all the teams, also !)

2003 Kaneko K, Terada K et al. (Japan)
2004 Miehe & Dettmar (Germany)
2009 Meyer et al. 2009 (Germany)
2010 Nitka, Desrues et al. (3SR,Grenoble, France)
2013, 2014,… Guo, Zhao (Hong-Kong)
2014 Nguyen, Desrues et al. (3SR,Grenoble, France)
2015 Liu, WaiChing et al. (USA)
2016 Shahin, Desrues et al. (3SR,Grenoble, France)
…

Principle

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



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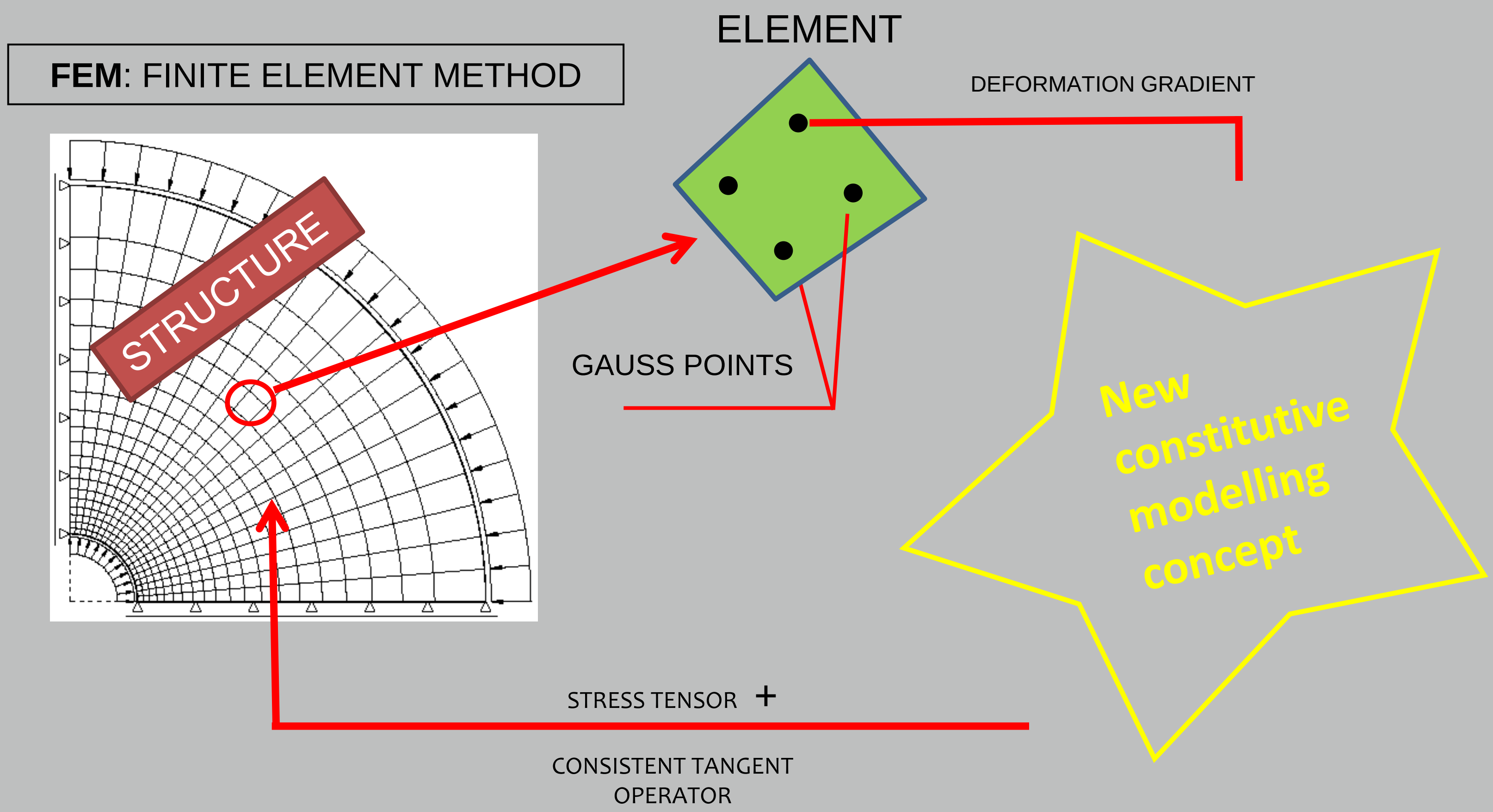

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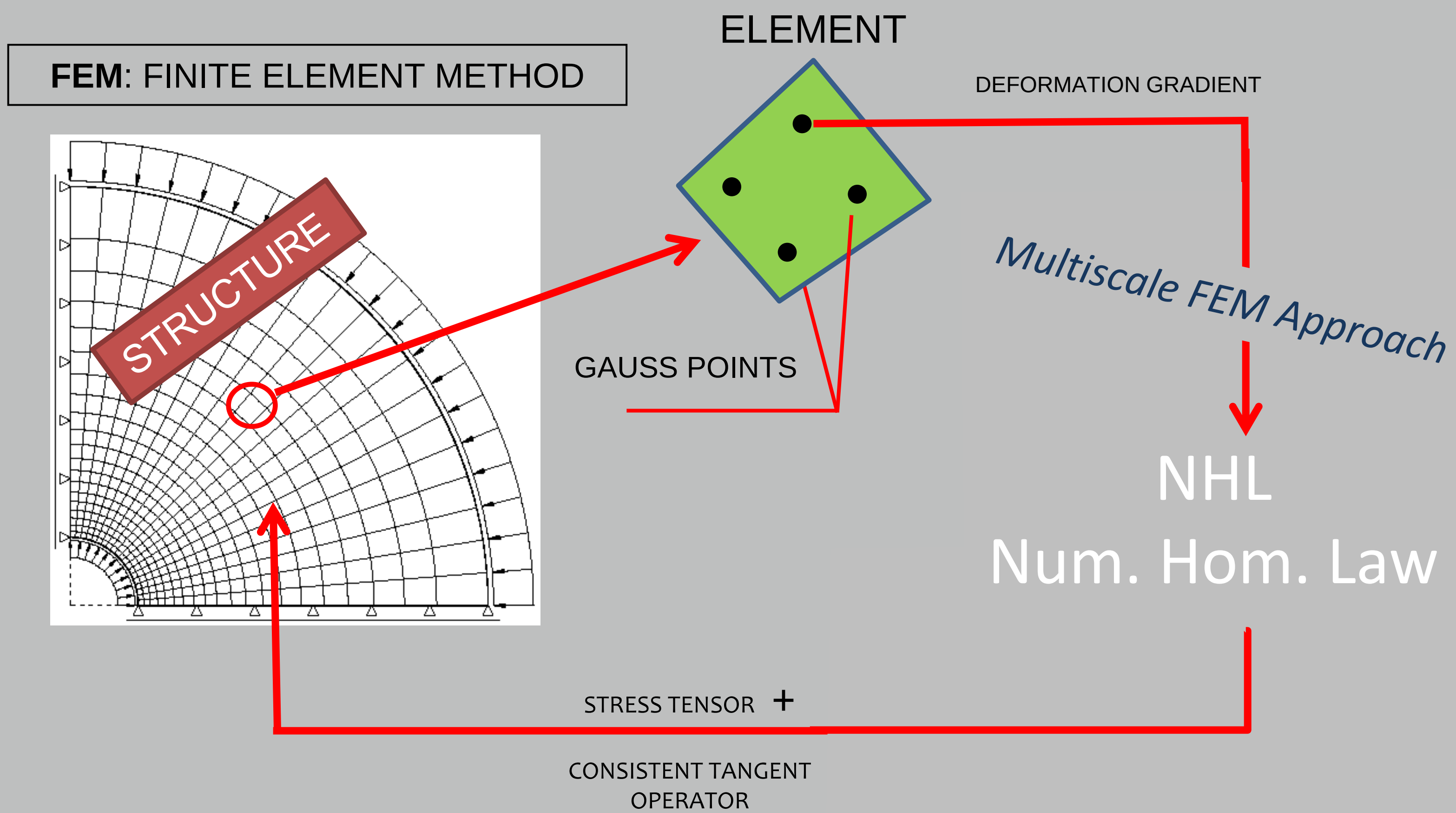
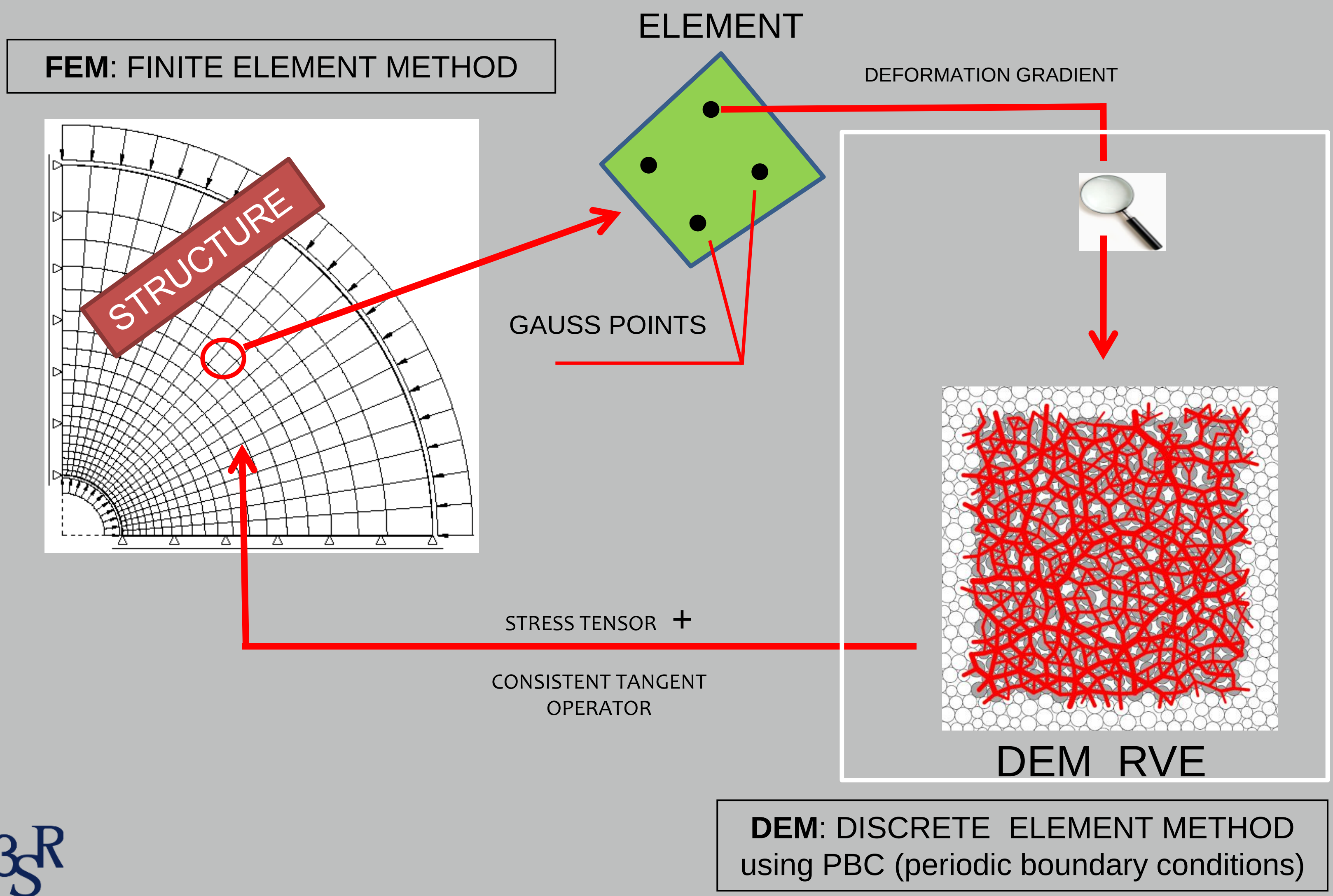


Principle

A two-scale numerical homogenization approach by FEM - DEM



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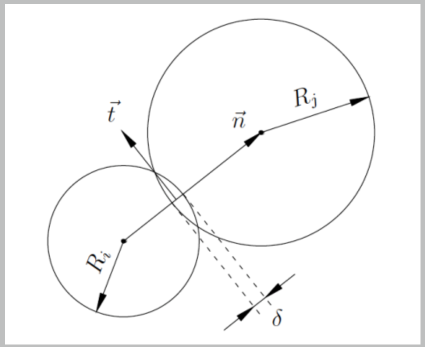
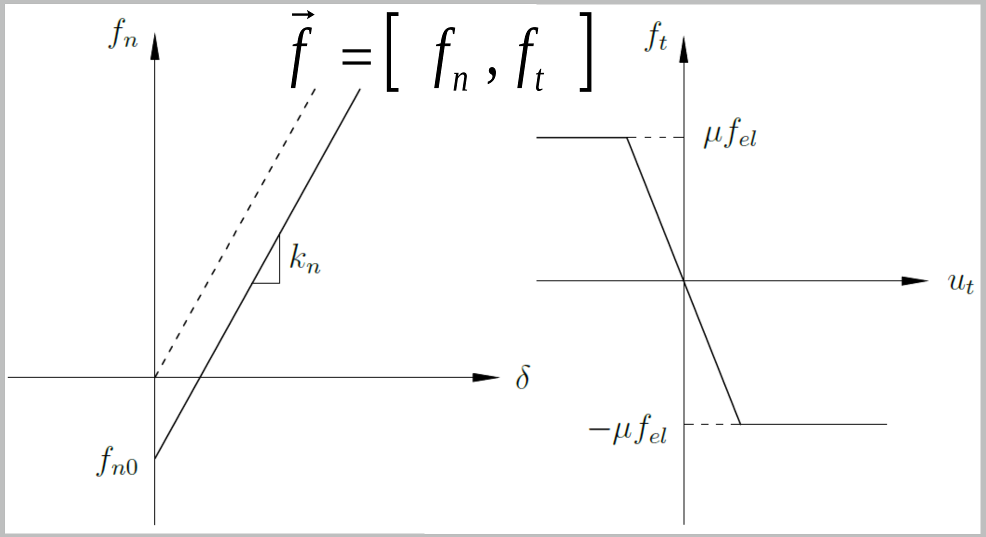
Micro-scale Model



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



Macroscopic 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

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

- 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)

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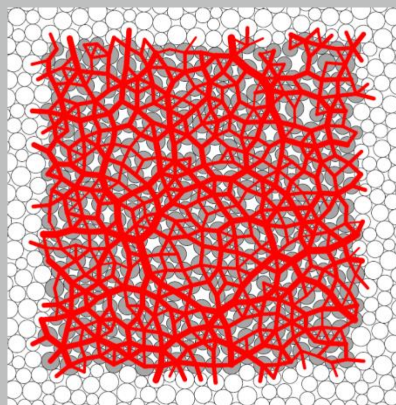
Micro-scale Model

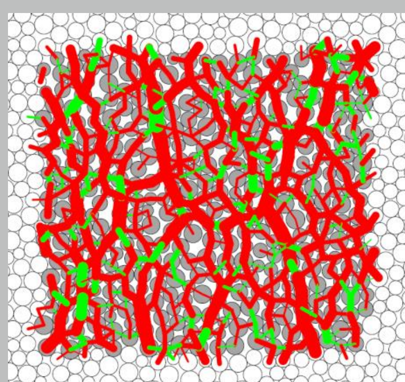
Biaxial test (DEM with PBC): REV contains 400 particles



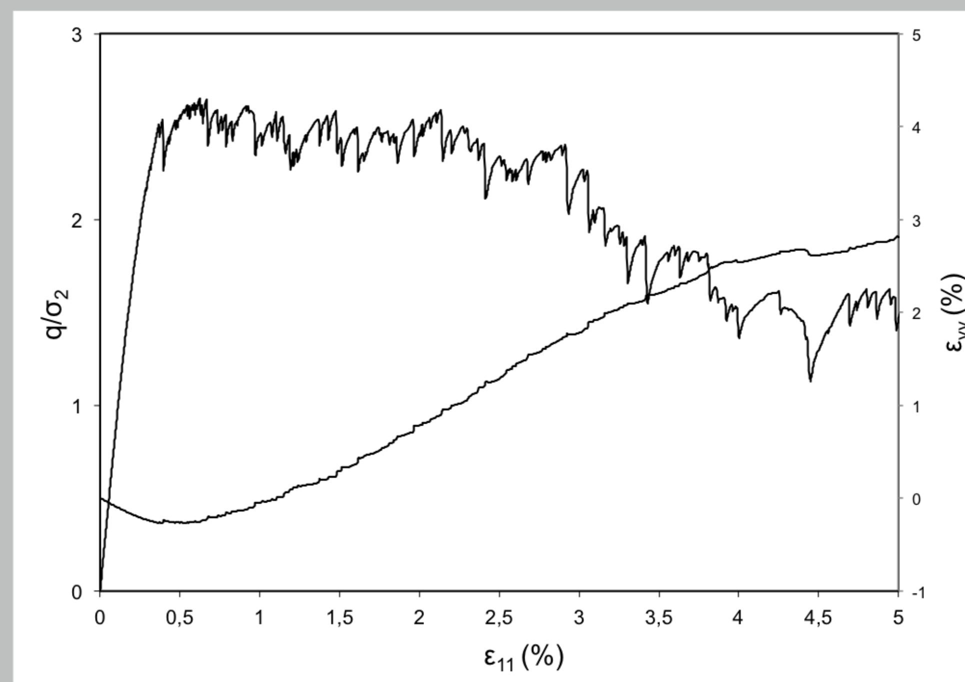
Initial configuration

— f_c effective

— $f_c = 0$



at 3% of axial strain (ε_{11})



Outline

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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)

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

Outline

1. Introduction : principle
2. Micro-scale (DEM) Model
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4. FEM-DEM at work : examples of simulations :
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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 ,**

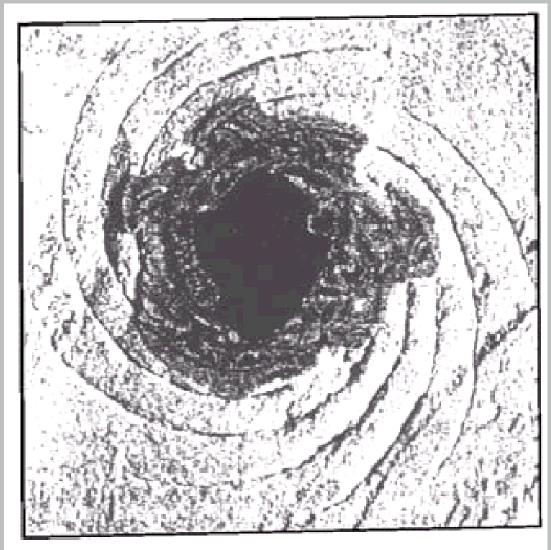
(can be studied as a hollow cylinder under differential pressure)

(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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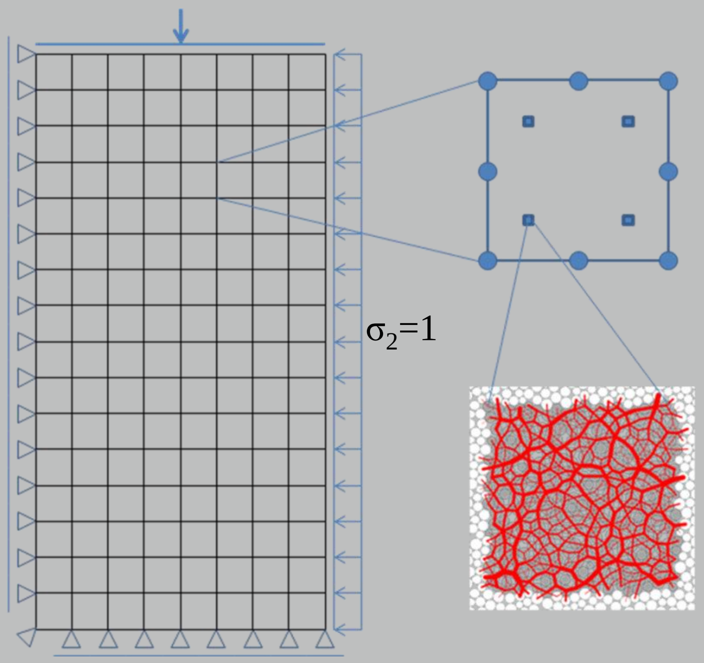
Multiscale Computations: Numerical results



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

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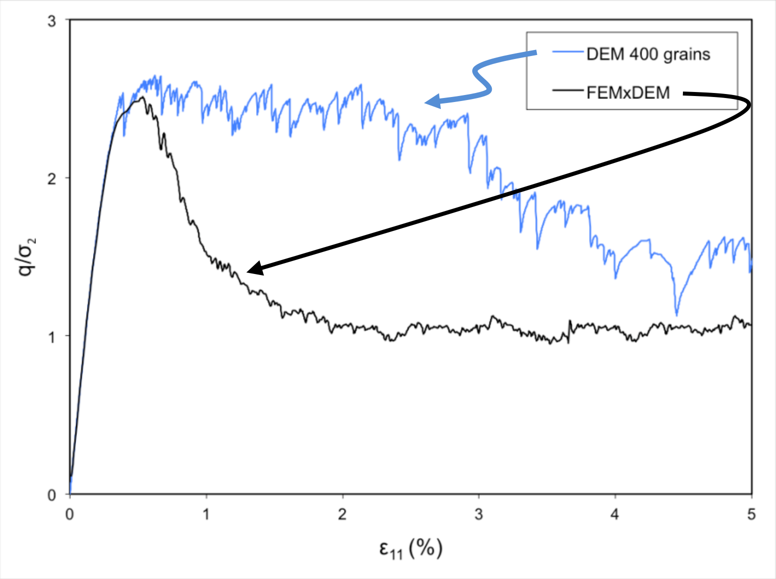
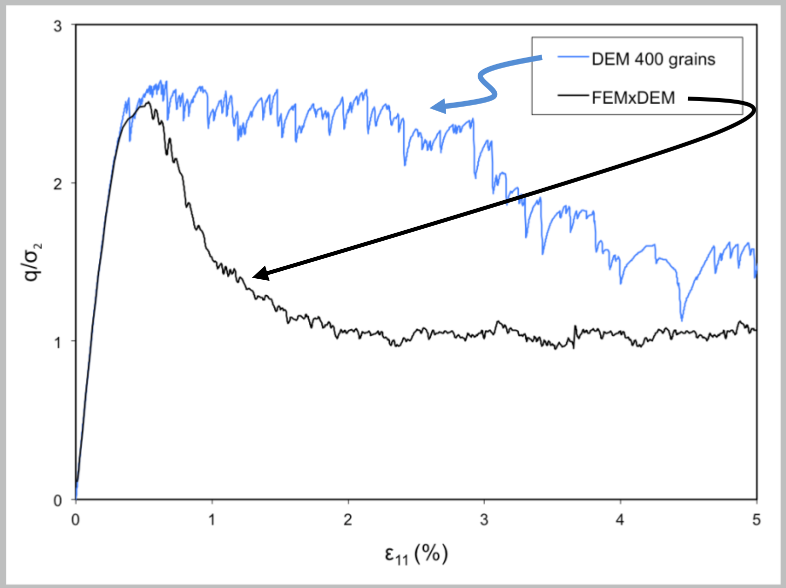
Strain Softening and Strain localization : FEM x DEM response

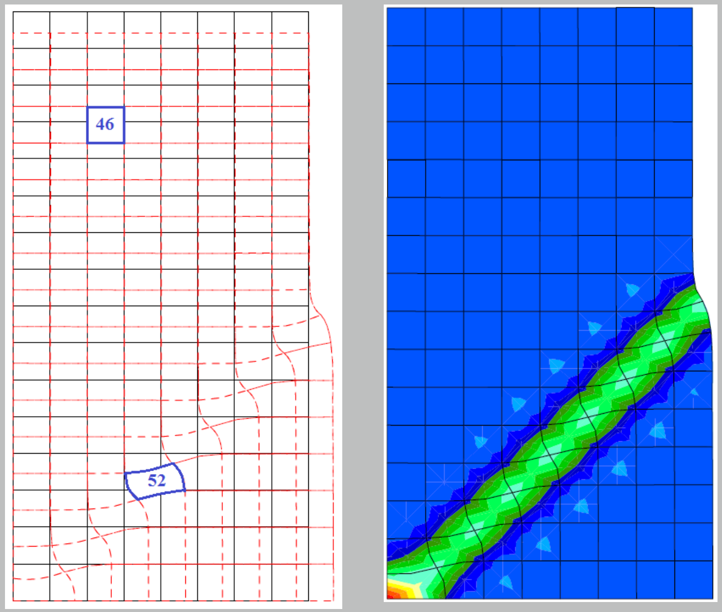


?? The response of the specimen modelled as a structure by FEMxDEM
differs considerably from the pure DEM response ??

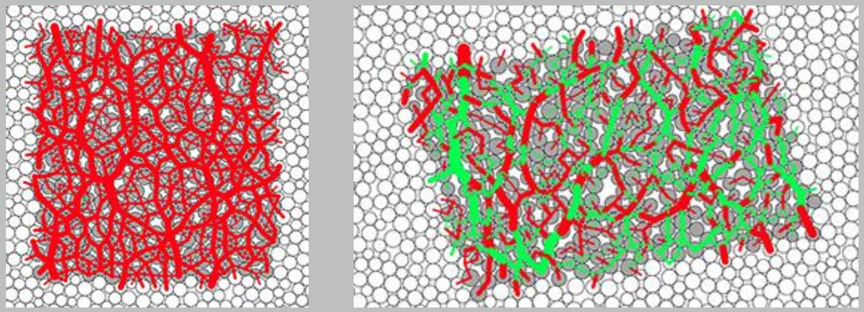
→ This is due to Strain localization in the structure

Strain Softening and Strain localization : FEM x DEM response





Deformed structure and second invariant of strain tensor



Element 46 Element 52

Deformed REV

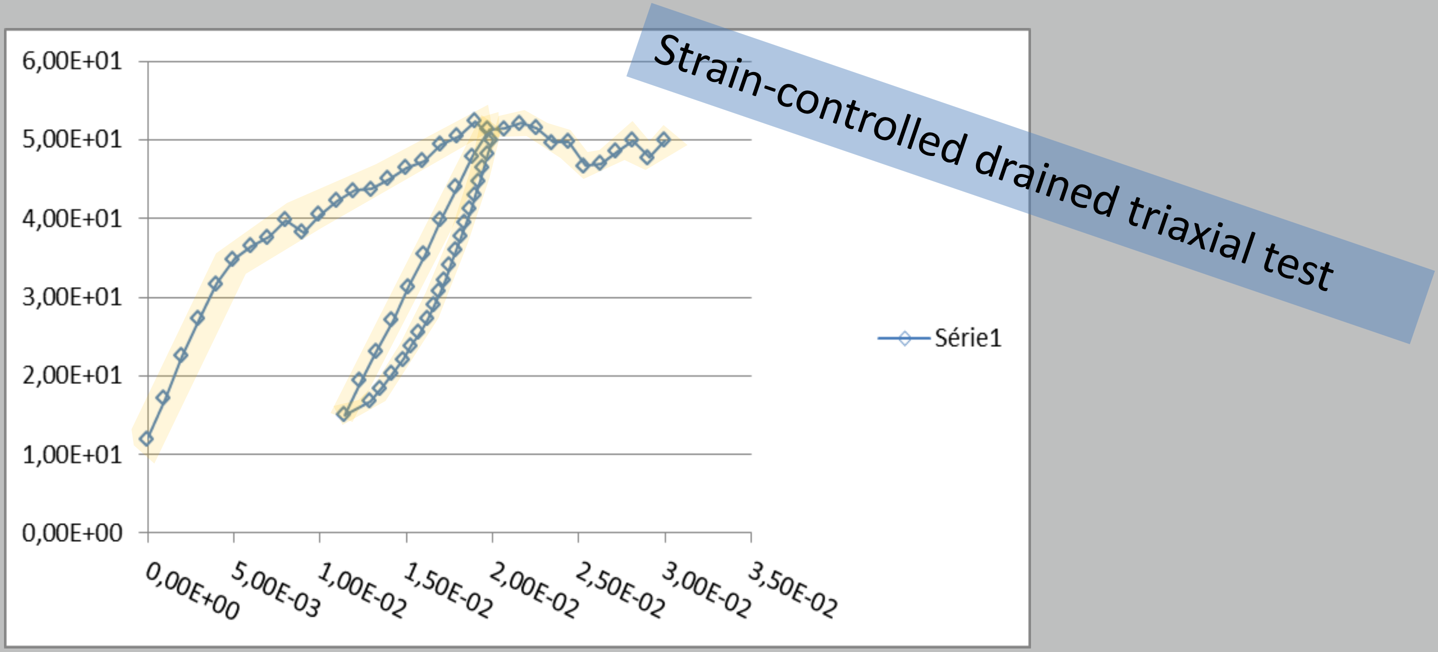
NHL-DEM performances :

- Strain softening and strain localisation

NHL-DEM performances :

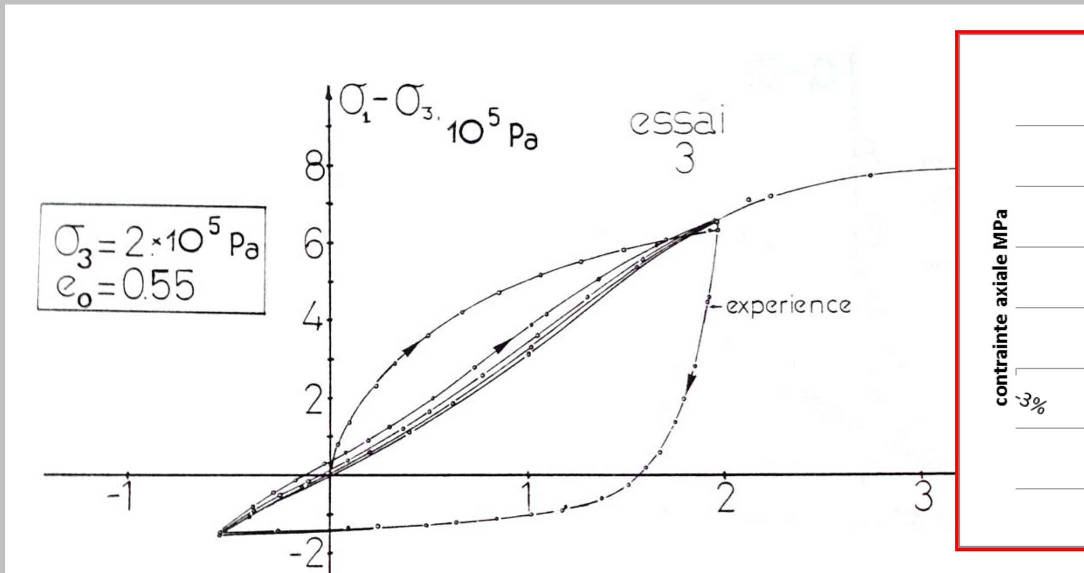
- Strain softening and strain localisation
- Cyclic response
- Anisotropy
- Principal stress rotations

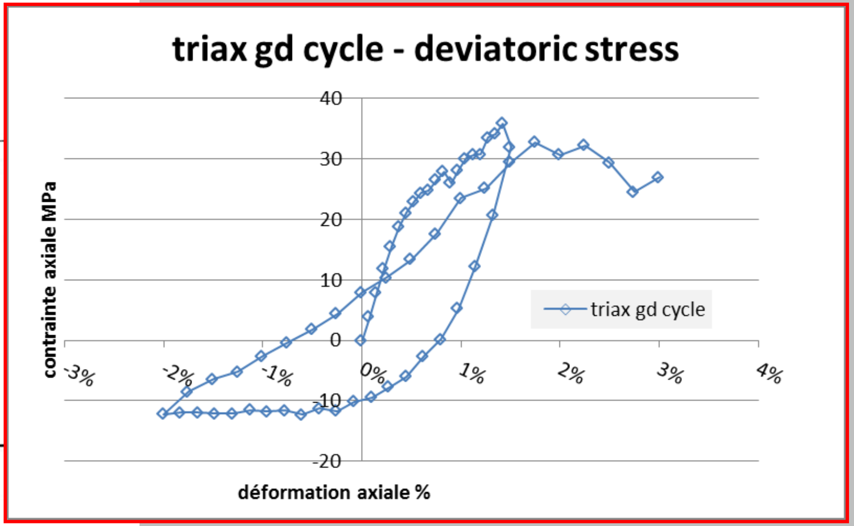
NHL-DEM performances : cycles



- Simple loading-unloading-reloading :
- The RVE state variables (grain's position, contacts and contact forces) retain all the information necessary to predict :
  - progressive stiffness degradation upon continuous loading,
  - then quasi-but-not-totally elastic unloading,
  - then elastic reloading
  - up to re-entering the plastic regime

NHL-DEM performances : compression-extension cycles





I. Thanopoulos (1981) "Contribution à l'étude du comportement cyclique des milieux pulvérulents", Thèse de Docteur-Ingénieur, Grenoble University

- Large compression-extension cycles :
  - Not impossible to model with formal CE, …but difficult
- NHL-DEM provide a **reasonably good** response …**without any special development**

NHL-DEM performances :

- Strain softening and strain localisation
- Cyclic response
- Anisotropy
- Principal stress rotations

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

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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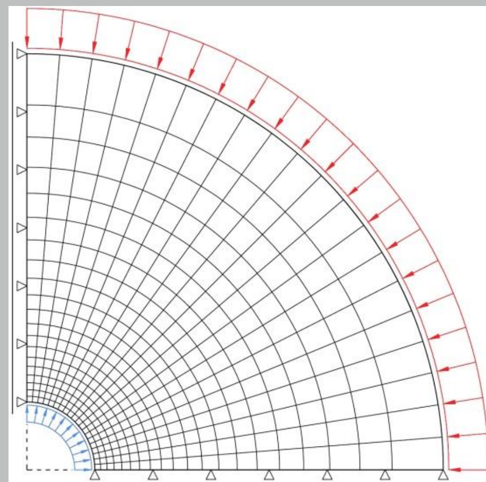
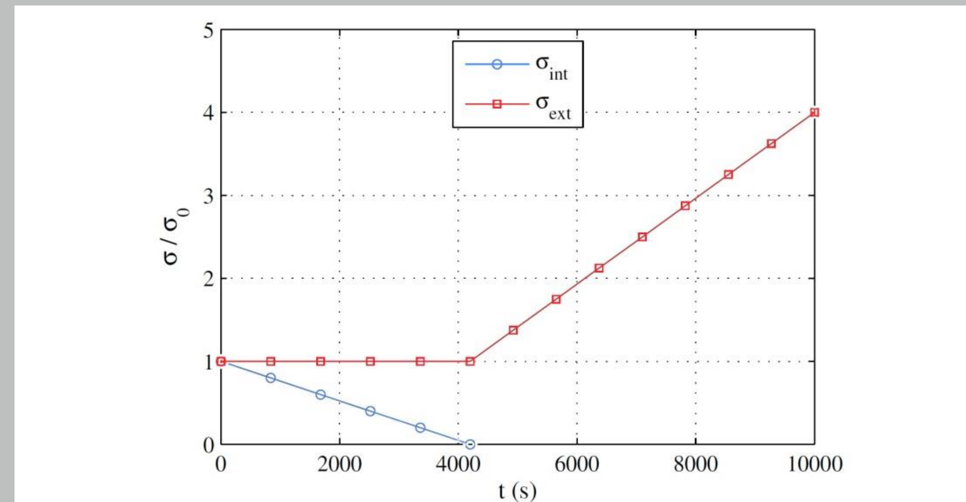
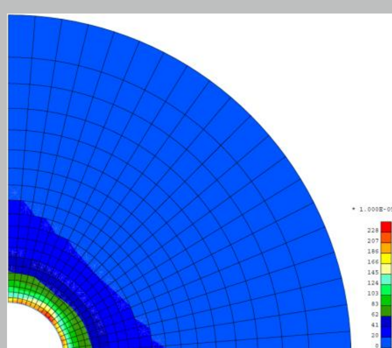
Multiscale Computations: Hollow cylinder (drilling), Strain localization

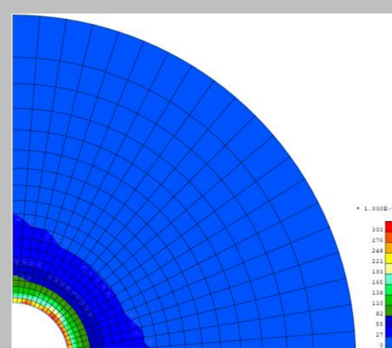




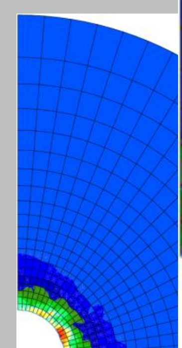
Deformed structure and second invariant of strain tensor



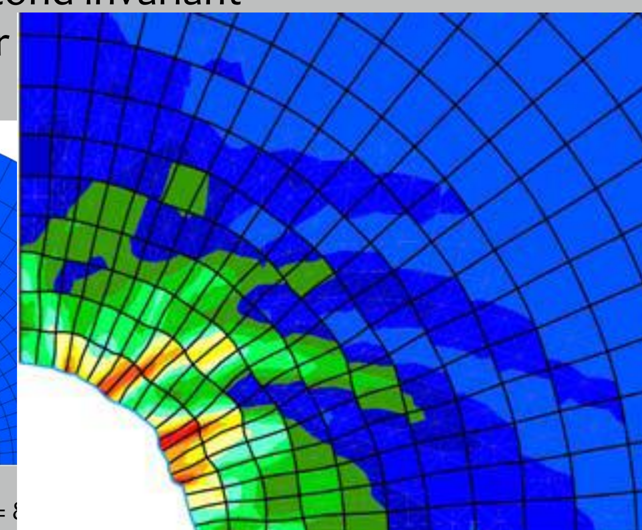
t = 3700
$\varepsilon_{equ\ max}$ = 228. 10^{-5}



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

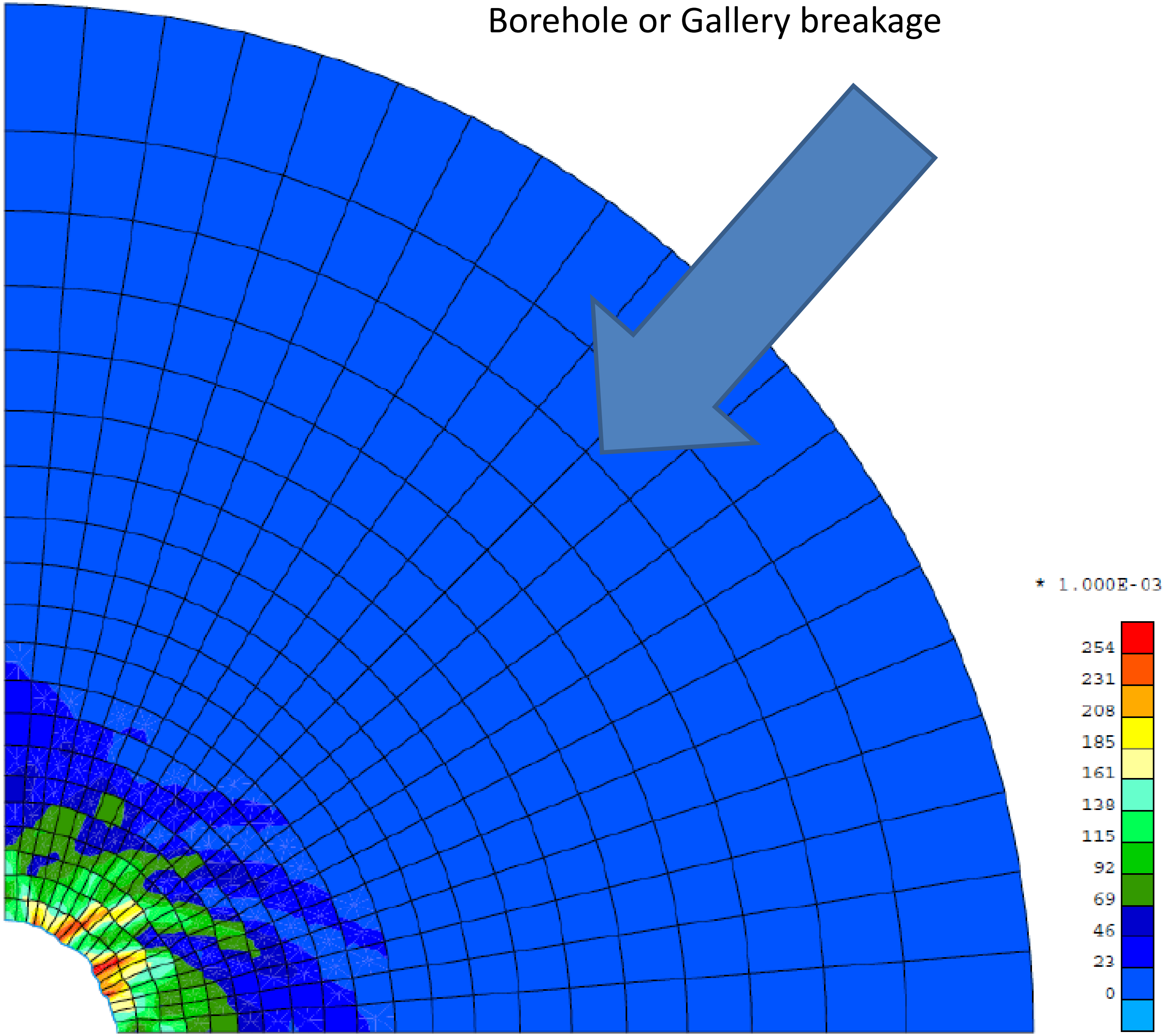


t =
$\varepsilon_{equ\ max}$ = 124. 10

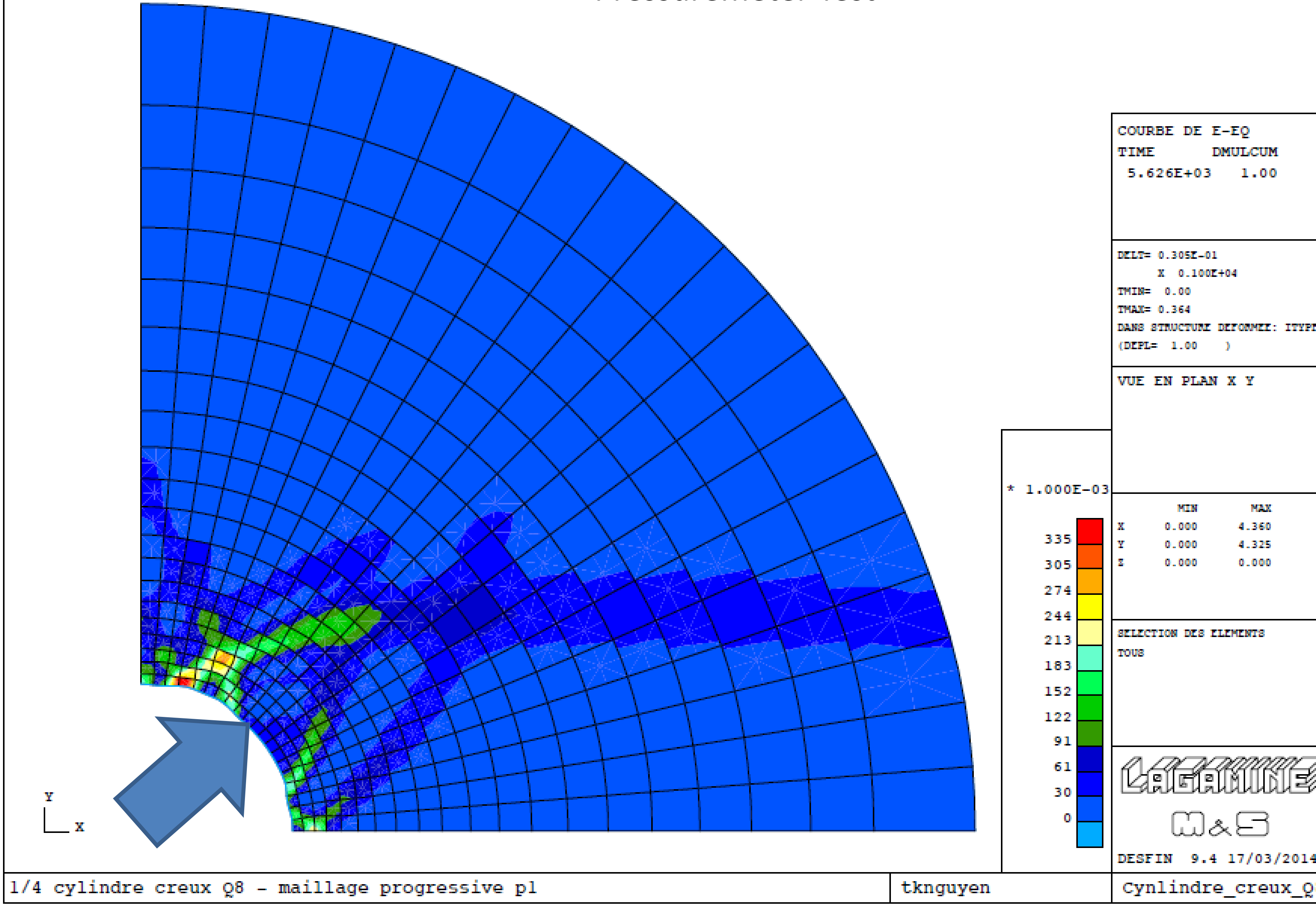


$\varepsilon_{equ\ max}$ = 254. 10

Borehole or Gallery breakage



Pressuremeter Test



Hollow cylinder inflation as a pressuremeter test

Cavity volume vs Pressure curve :

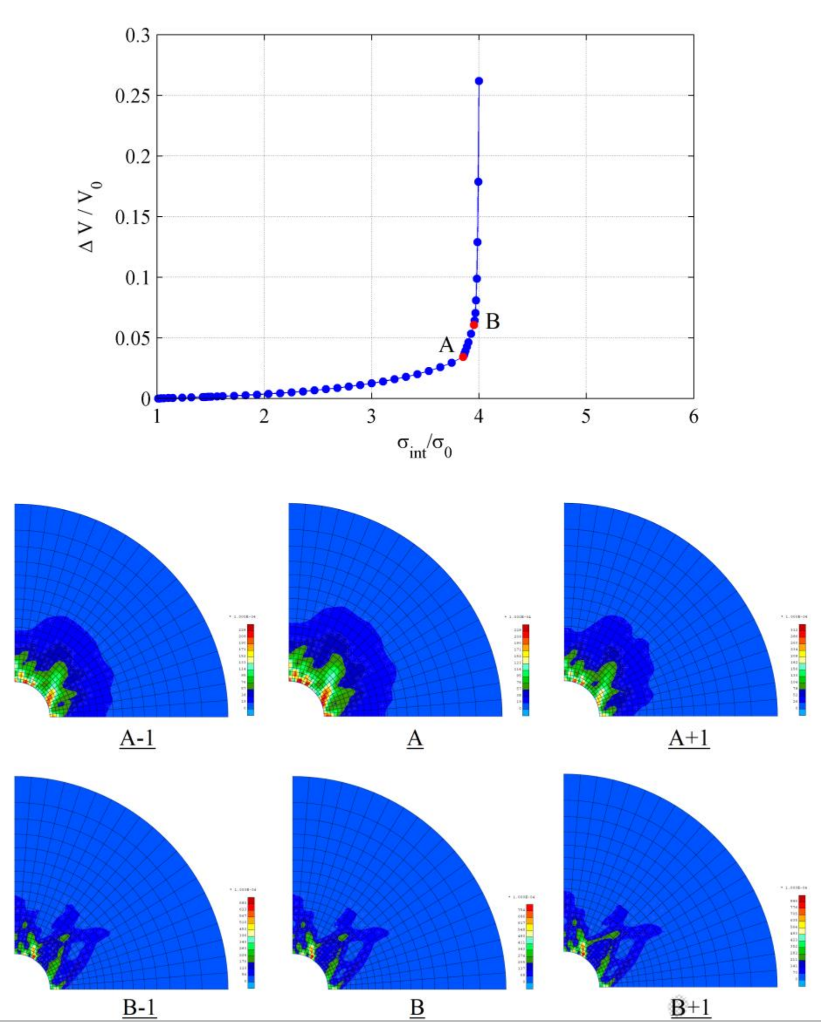
Typical features of the **pressuremeter log curve** :

Initial quasi linear phase,

(*pressuremeter module*)

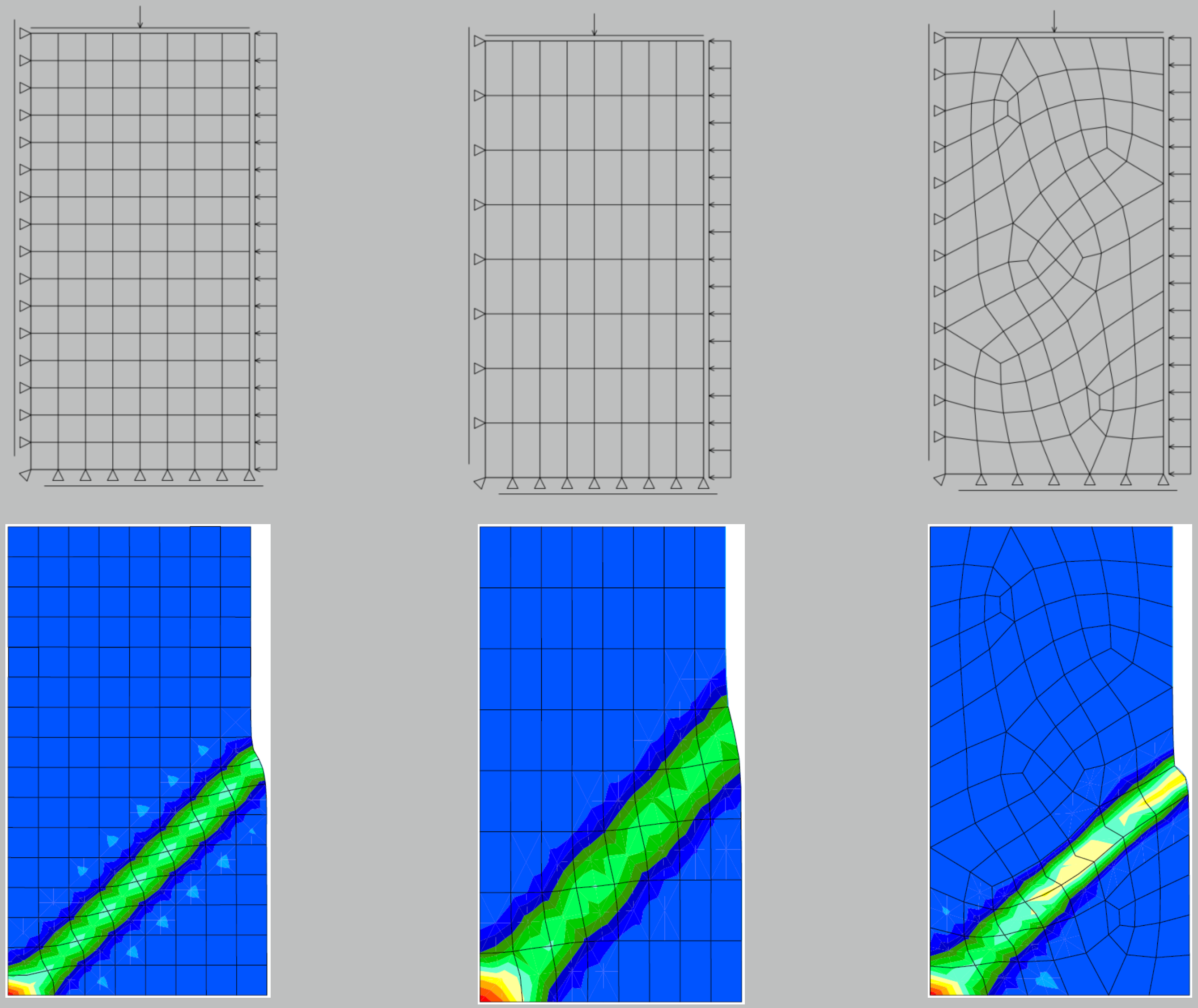
Then transition to a vertical assymptot *(so called limit pressure*)

Localisation effect : quasi discontinuous transition from the quasi linear phase to the final vertical branch (point A)



Multiscale Computations: different meshes

!!! Mesh dependency (as usual in FEM) : issues and solutions



128 elements

64 elements

106 elements

(partial) Conclusions

First CONCLUSION :

- We have presented an ***integrated 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.
- 2^{nd} **gradient regularization** allows to restore mesh *independency*
- **Parallelisation (OpenMP / MPI)** allows to mitigate the CPU cost issue *:*
  - Parallelisation of the code (element loop) using **OpenMP** has showed to be very effective : scalability about 80%, but shared memory → limited number of processors
  - Parallelisation using **MPI** even more effective since a priori no limit is set to the number of processors : excellent scalability as well, improving with the size of the micro problem

PERSPECTIVES

-3D approach

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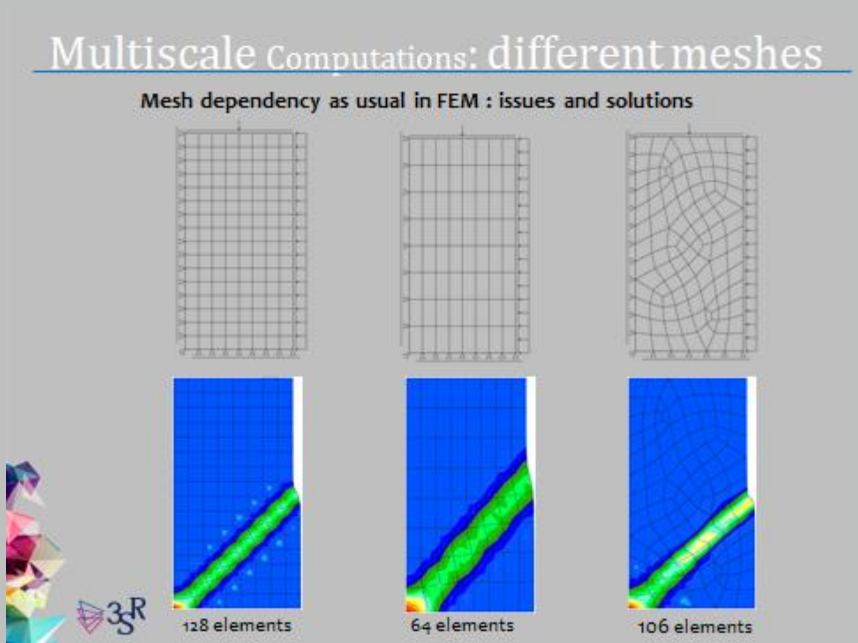
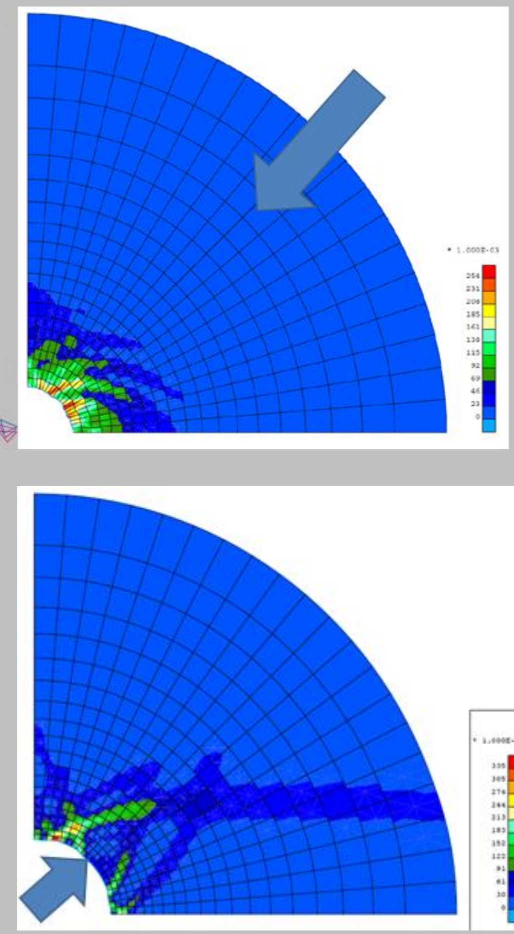
Mesh dependency problem

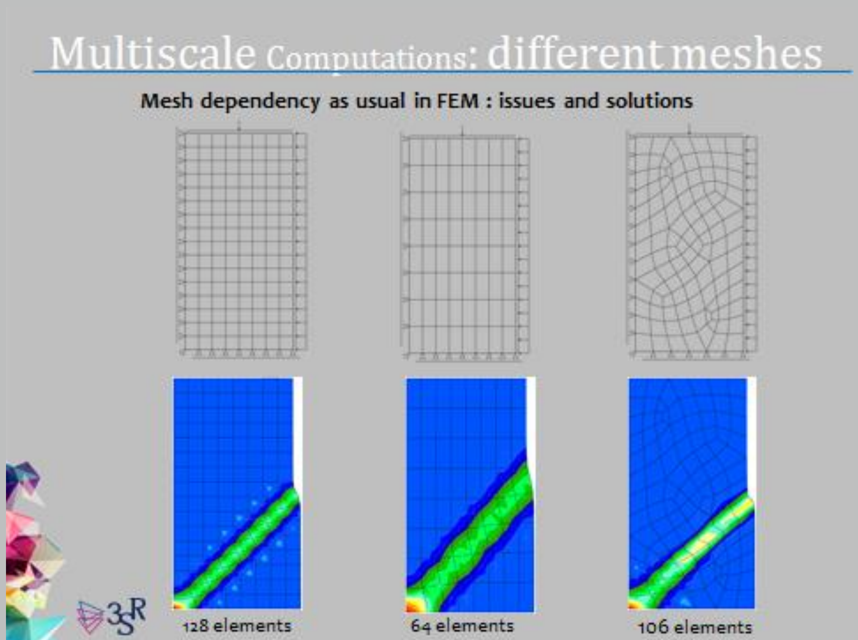


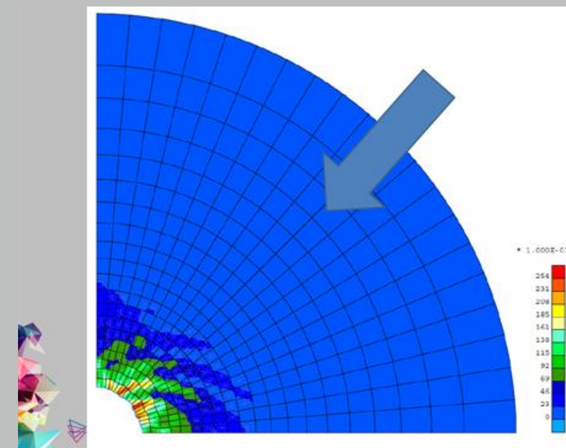


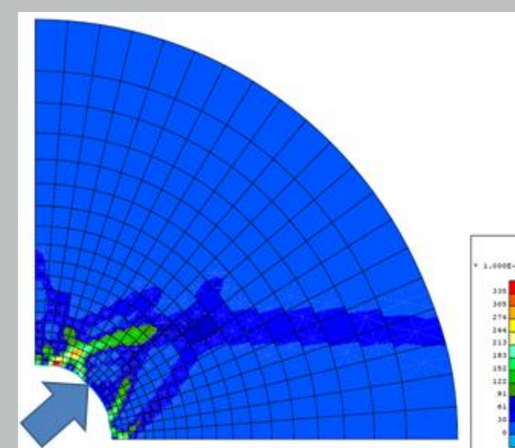
Same problem in borehole / pressuremeter

Mesh dependency problem

Solution ?
: regularization of the bvp

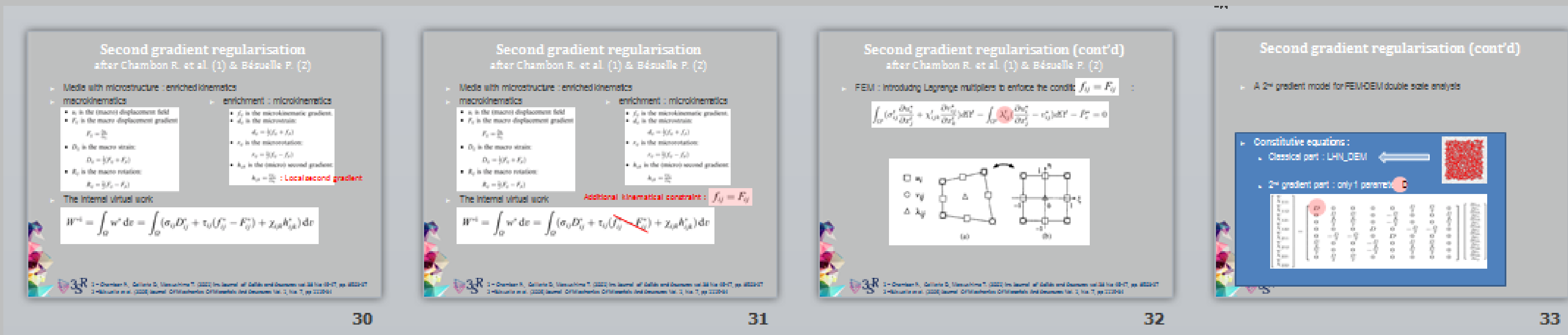






2nd gradient regularisation

- What is it ? … a brief *aperçu* in 4 slides



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 virtual internal work :

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

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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    $$r_{ij} = \frac{1}{2}(f_{ij} - f_{ji})$$

  - h_{ijk} is the (micro) second gradient:

    $$h_{ijk} = \frac{\partial f_{ij}}{\partial x_k}$$

- The virtual internal work :

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

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

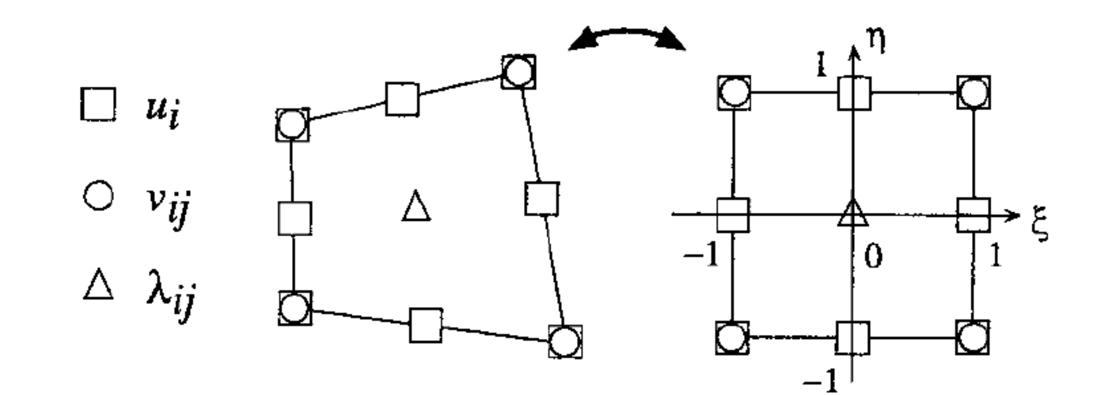
1 – Chambon R., Caillerie D., Matsushima T. (2001) **Int. Journal of Solids and Stuctures v**ol.38 No 46-47, pp. 8503-27
2 –Bésuelle, Chambon et al. (2006) **Journal Of Mechanics Of Materials And Structures** Vol. 1, No. 7, pp 1115-34

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)

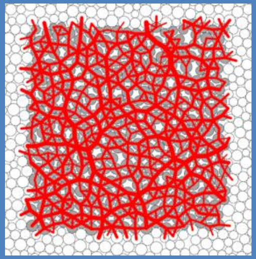
1 – Chambon R., Caillerie D., Matsushima T. (2001) **Int. Journal of Solids and Stuctures v**ol.38 No 46-47, pp. 8503-27

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

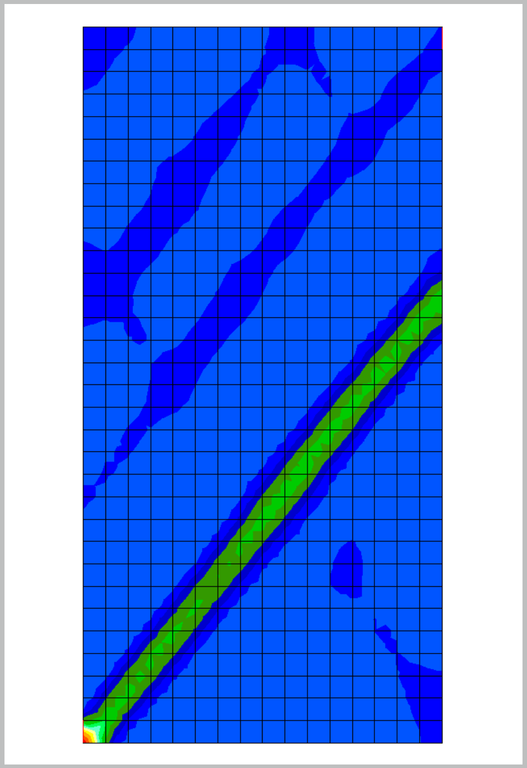
- **Constitutive equations :**
  - Classical part : LHN_DEM
  - 2nd gradient part : only 1 parameter D



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

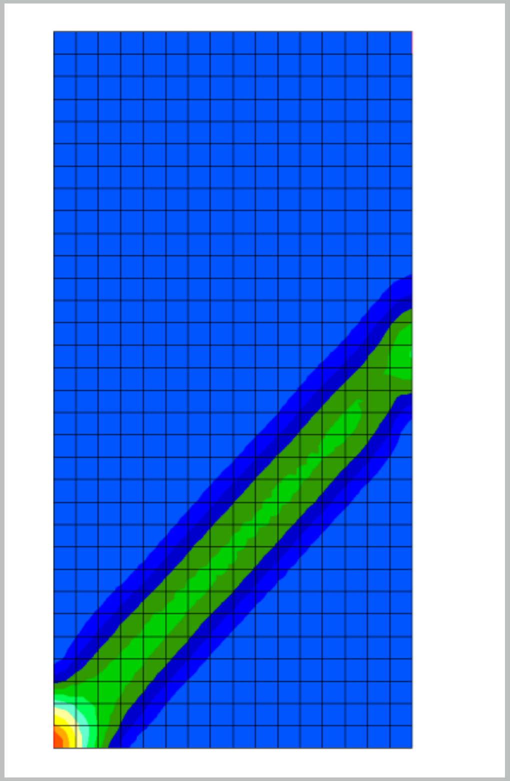
Restoring mesh independency with 2nd gradient

- No 2nd gradient



512 FE x 400 DE

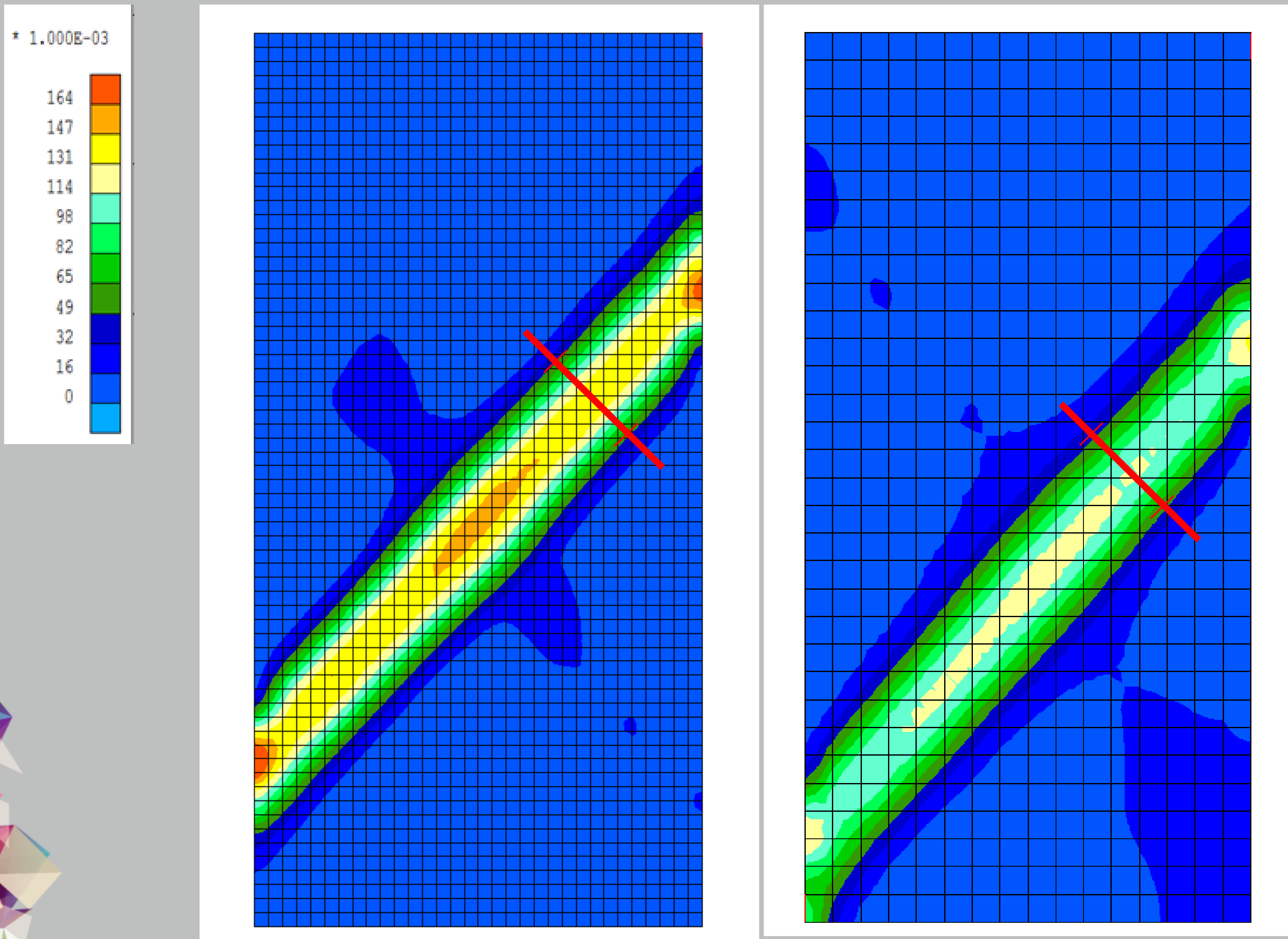
- With 2nd gradient



512 FE x 400 DE

Second Gradient D=0,64E-2

Axial strain = 2. 10-2

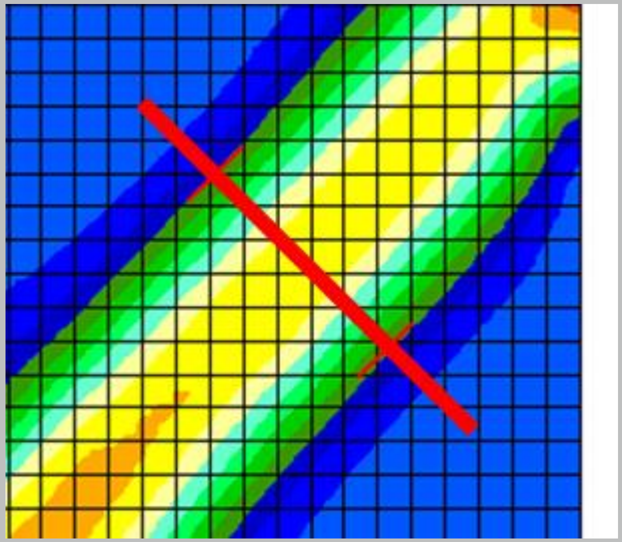


2048FEMx400DEM

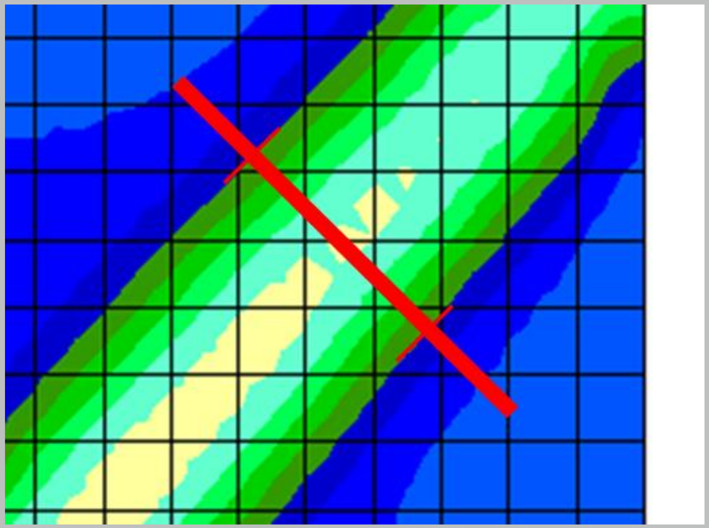
512FEMx400DEM

Restoring mesh independency with 2nd gradient

Second Gradient D=0,64E-2



2048 FE x 400 DE



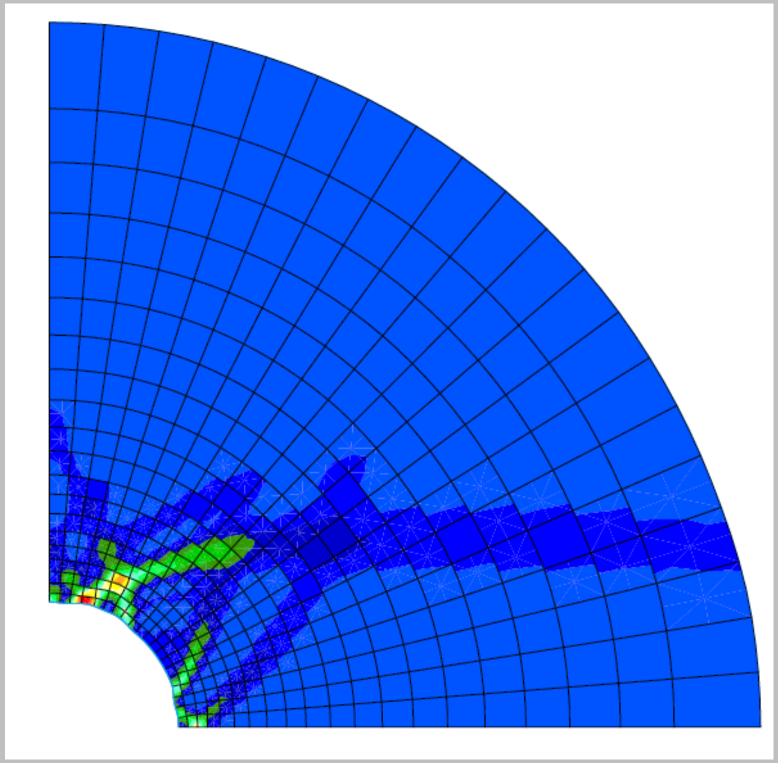
512 FE x 400 DE

2048FEMx400DEM

512FEMx400DEM

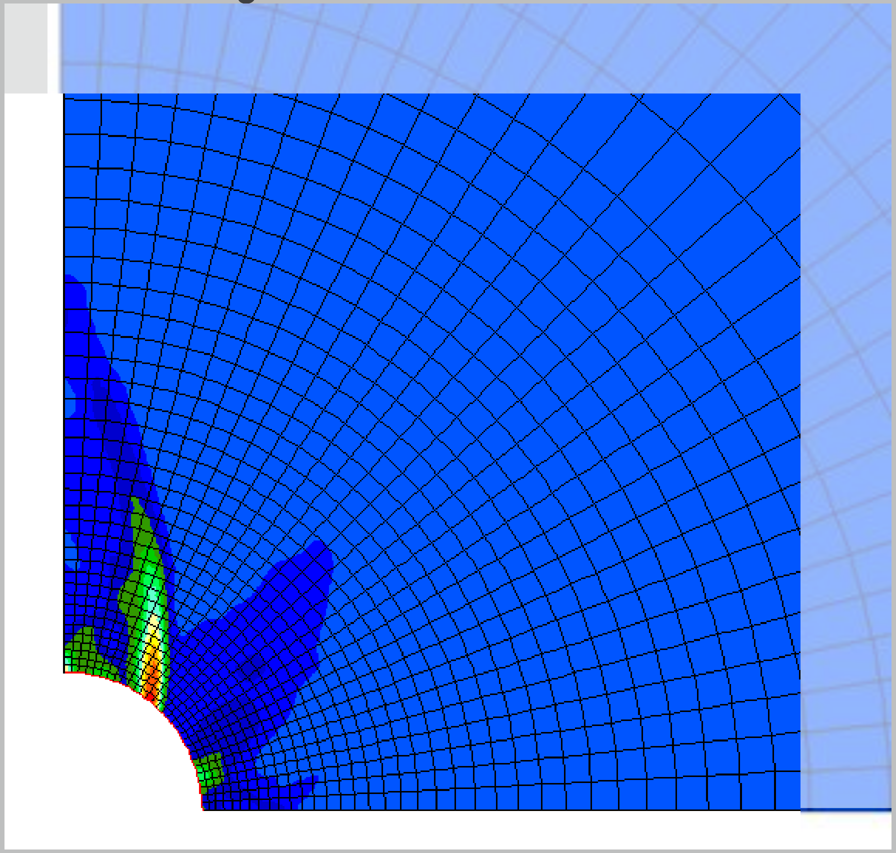
Restoring mesh independency with 2nd gradient

- No 2nd gradient



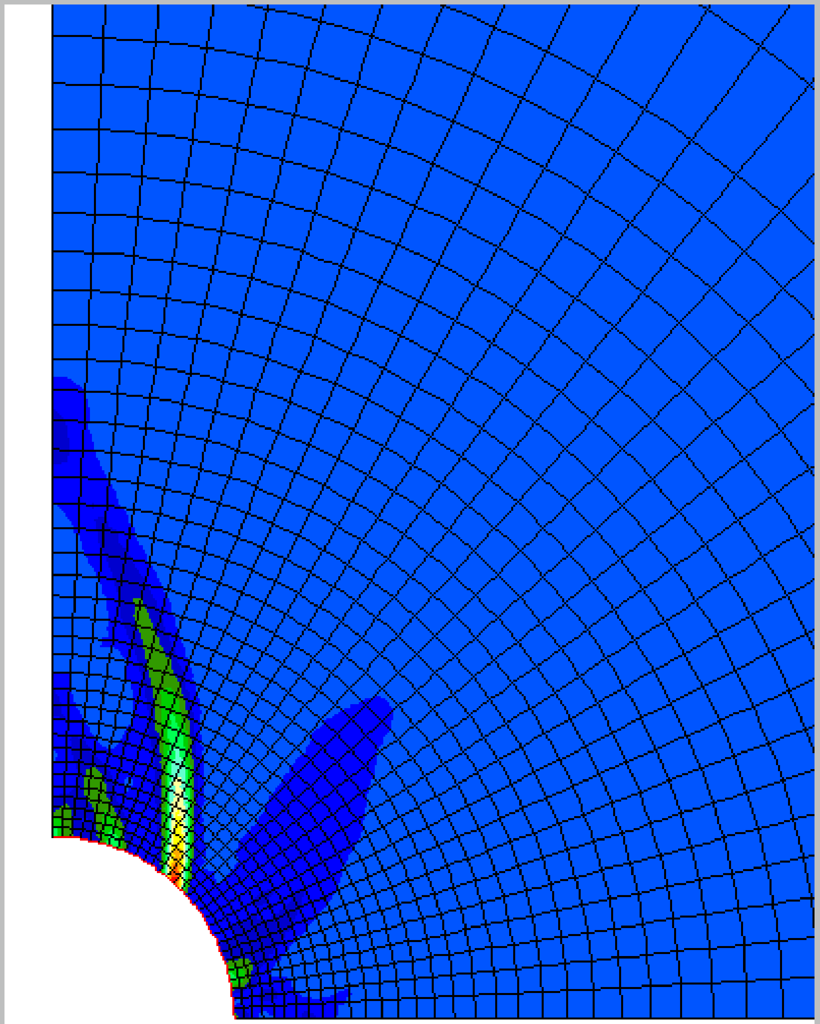
400 FE x 400 DE

- With 2nd gradient

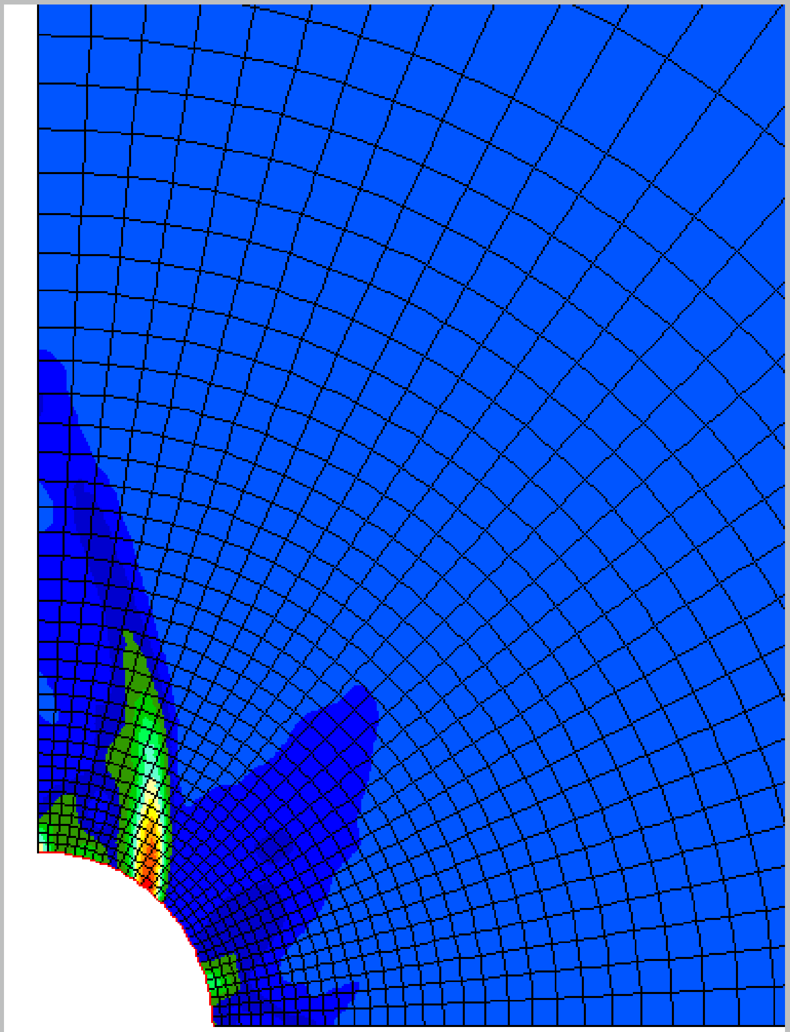


1230 FE x 400 DE

1290FEMx400DEM   - increase internal pressure



Second Gradient D=5,00E-2



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

(partial) Conclusions

Second CONCLUSION

- We have presented an ***integrated 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*

- **Parallelisation (OpenMP / MPI)** allows to mitigate the CPU cost issue *:*
    - Parallelisation of the code (element loop) using **OpenMP** has showed to be very effective : scalability about 80%, but shared memory → limited number of processors
    - Parallelisation using **MPI** even more effective since a priori no limit is set to the number of processors : excellent scalability as well, improving with the size of the micro problem

PERSPECTIVES

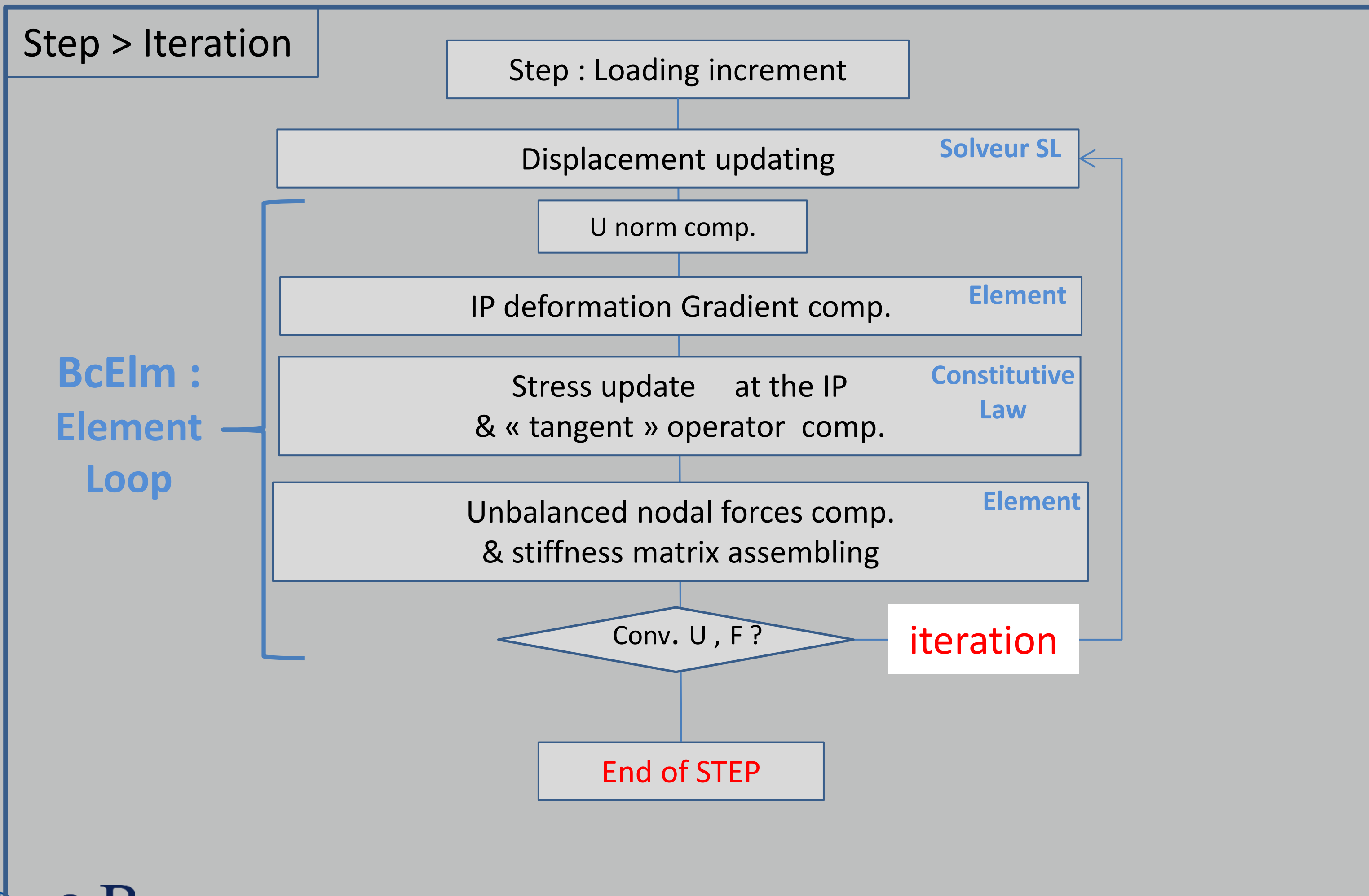
-3D approach

Outline

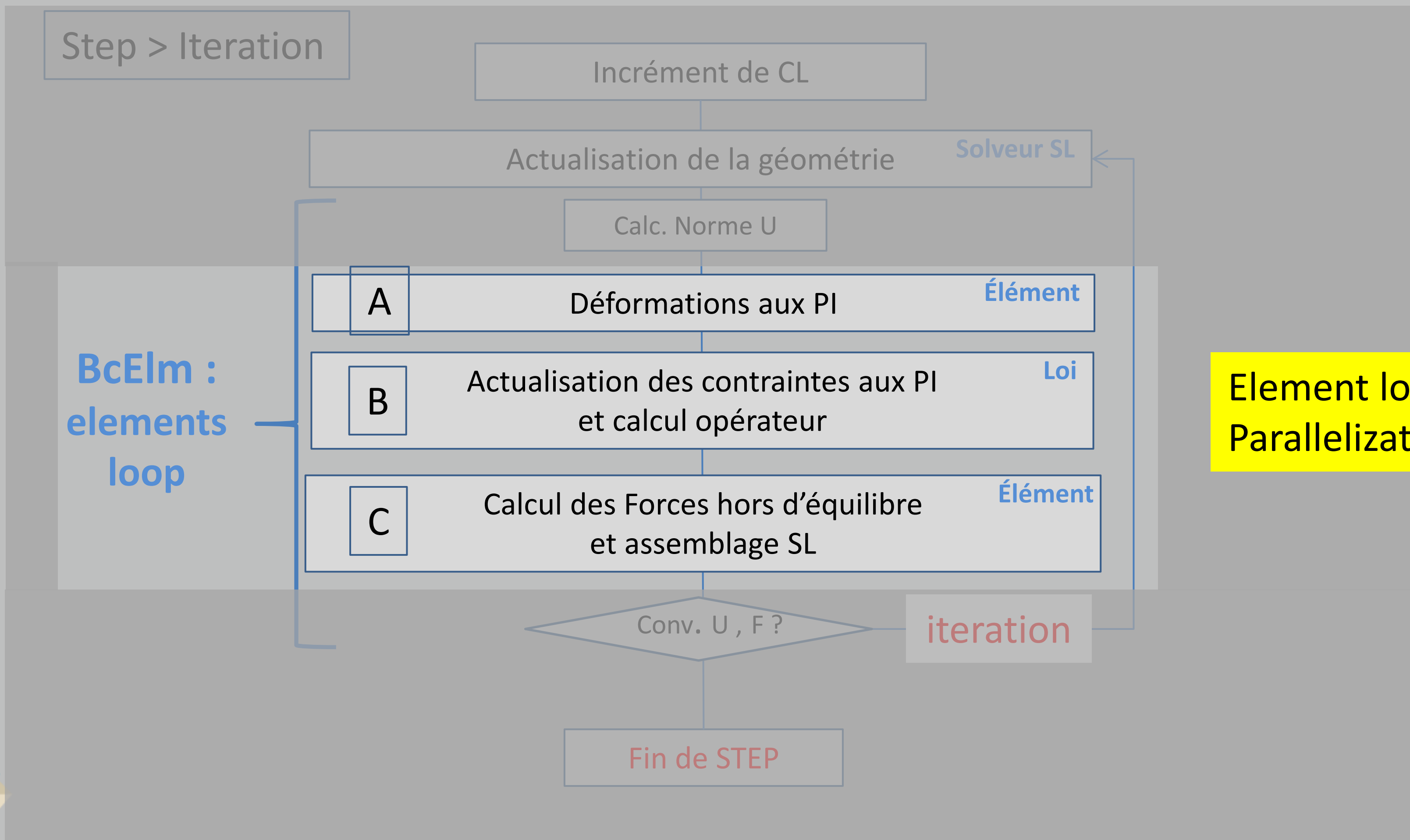
Computional efficiency : the CPU cost Issue

- Overcoming the CPU cost issue is a key point for practical use of double scale FEMxDEM analysis
- Enhancing the computational efficiency rely on several improvement tracks :
  - Choice of the Newton Raphson iteration operator
  - (2^{nd} gradient regularization)
  - Parallelization

FEM code workflow
(nothing new here)



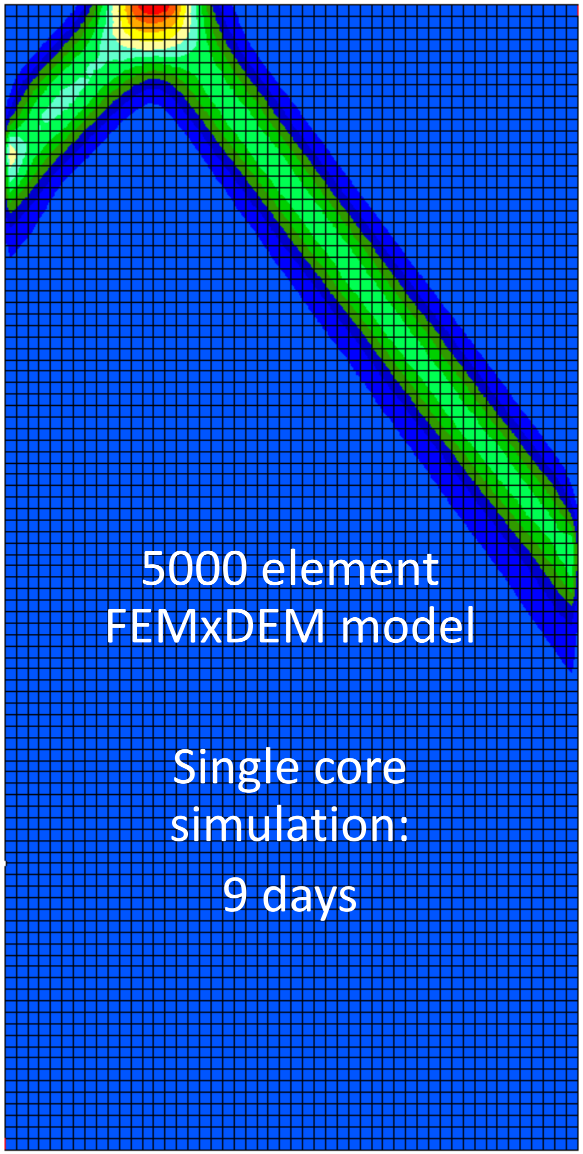
Element loop workflow



Element loop Parallelization

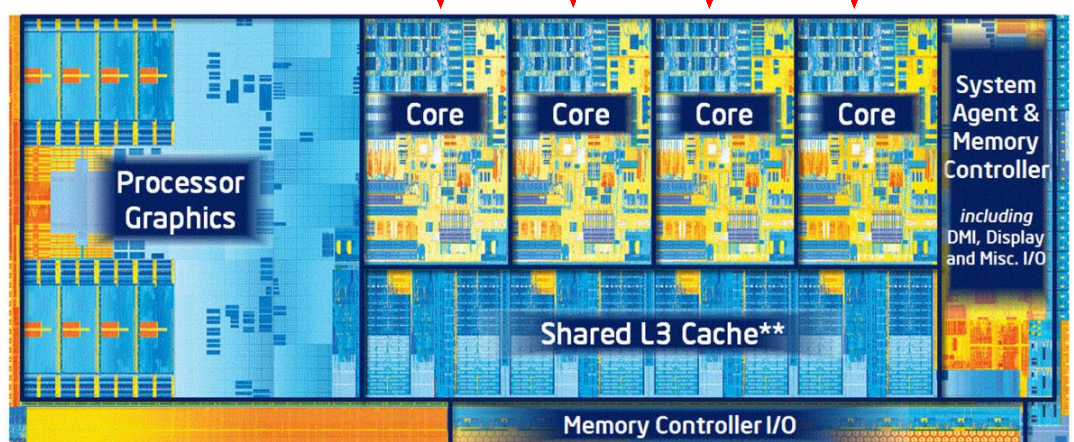
Element loop parallelisation

- Double scale → element intensive model.
- Parallelisation using an OpenMP : **shared memory model**
- Results: speedup up to 9 using a 12 core machine.
- Other approaches: massive parallelization (MPI).

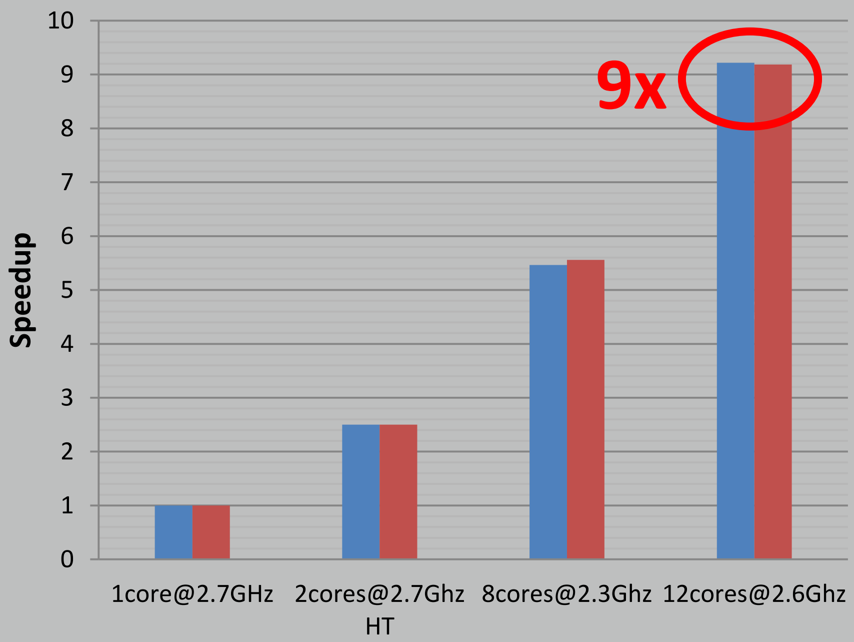


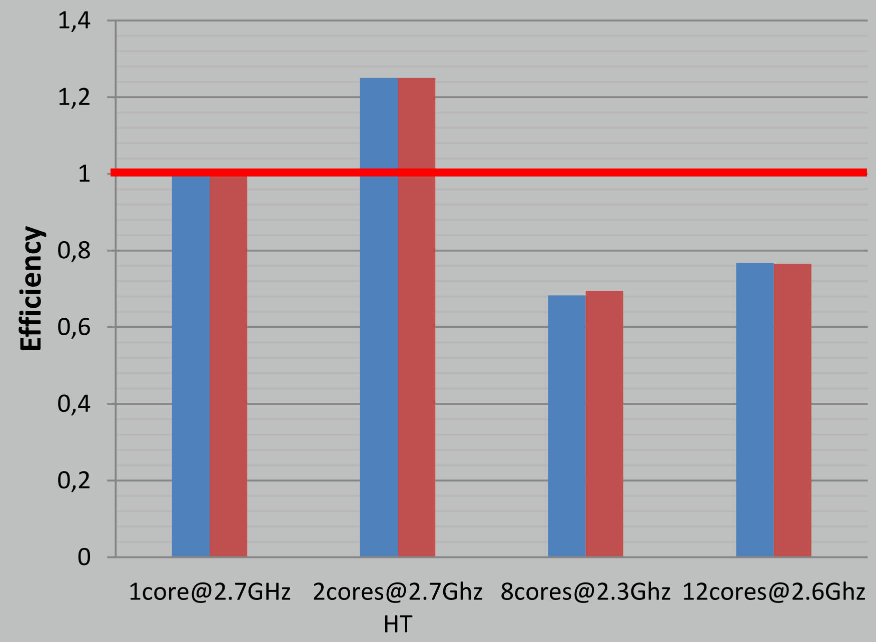
Element loop queue

OpenMP paradigm



Element loop parallelisation, performance

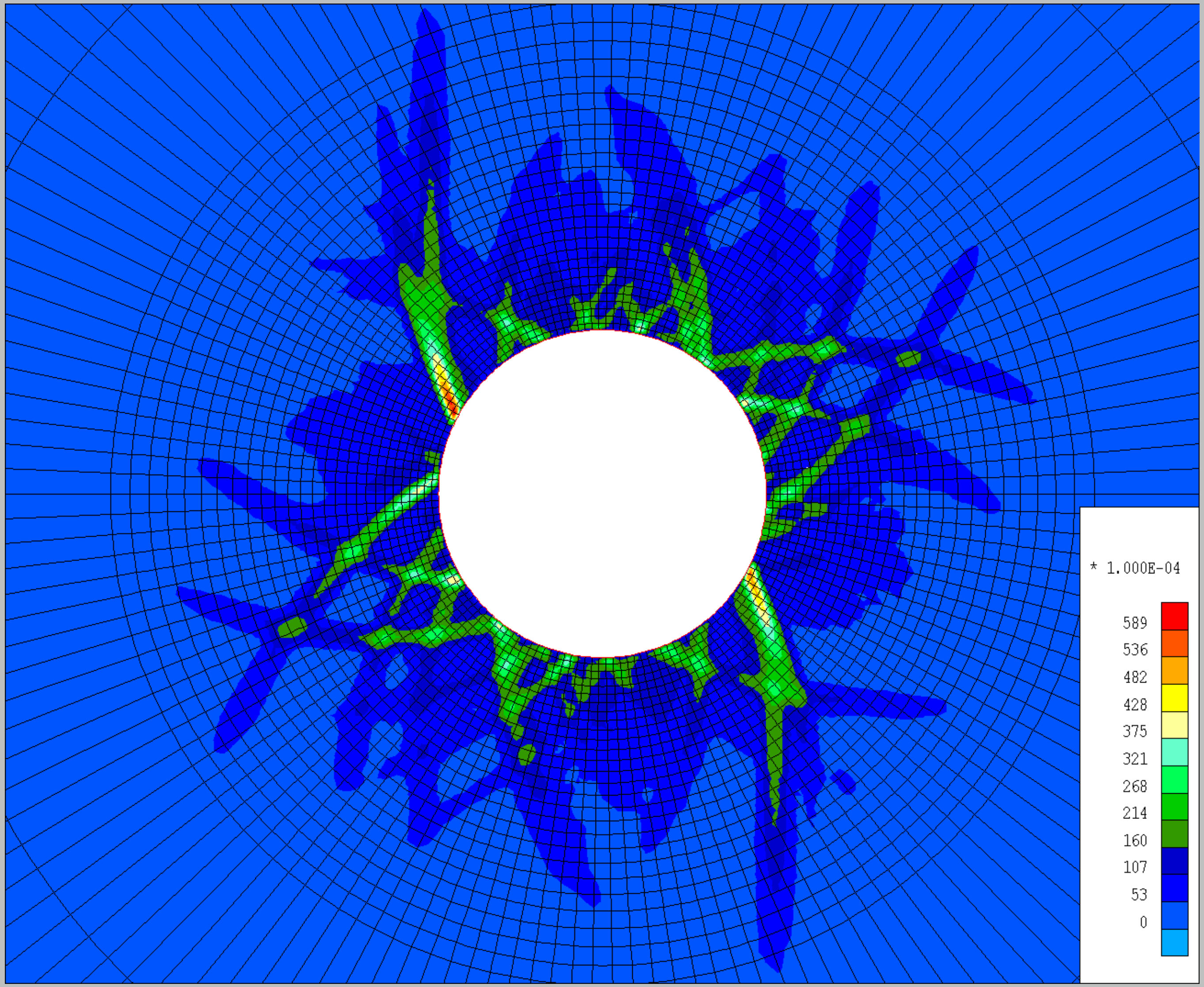




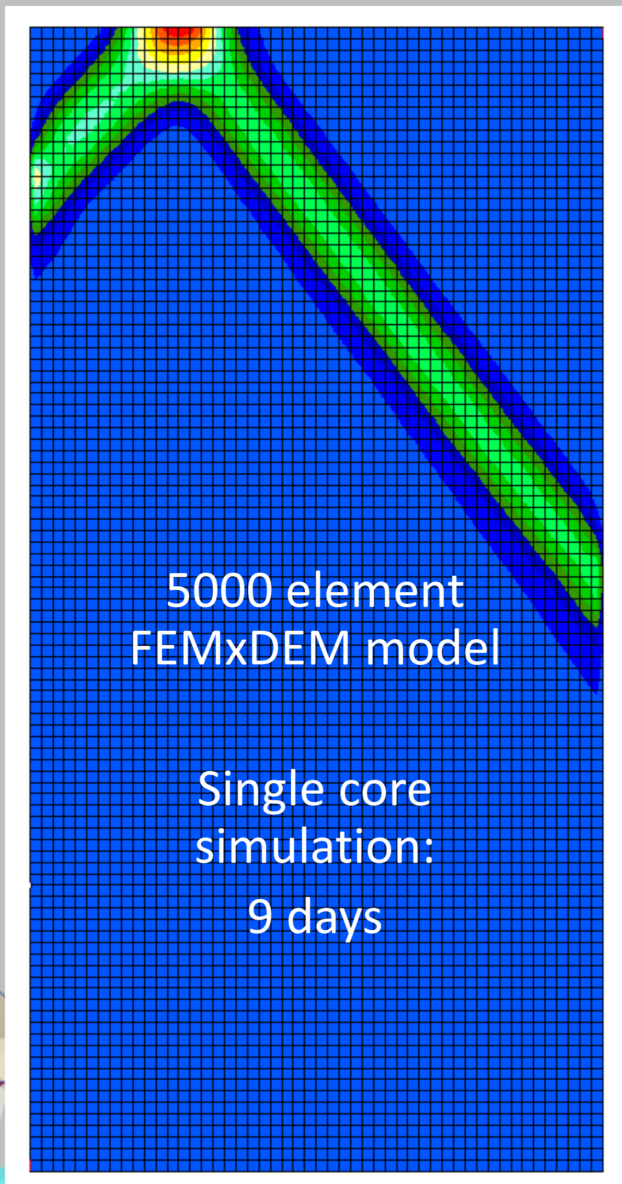
512 FEM x 400 DEM

2048 FEM x 100 DEM

Parallelisation : Computations with rather refined meshes become possible



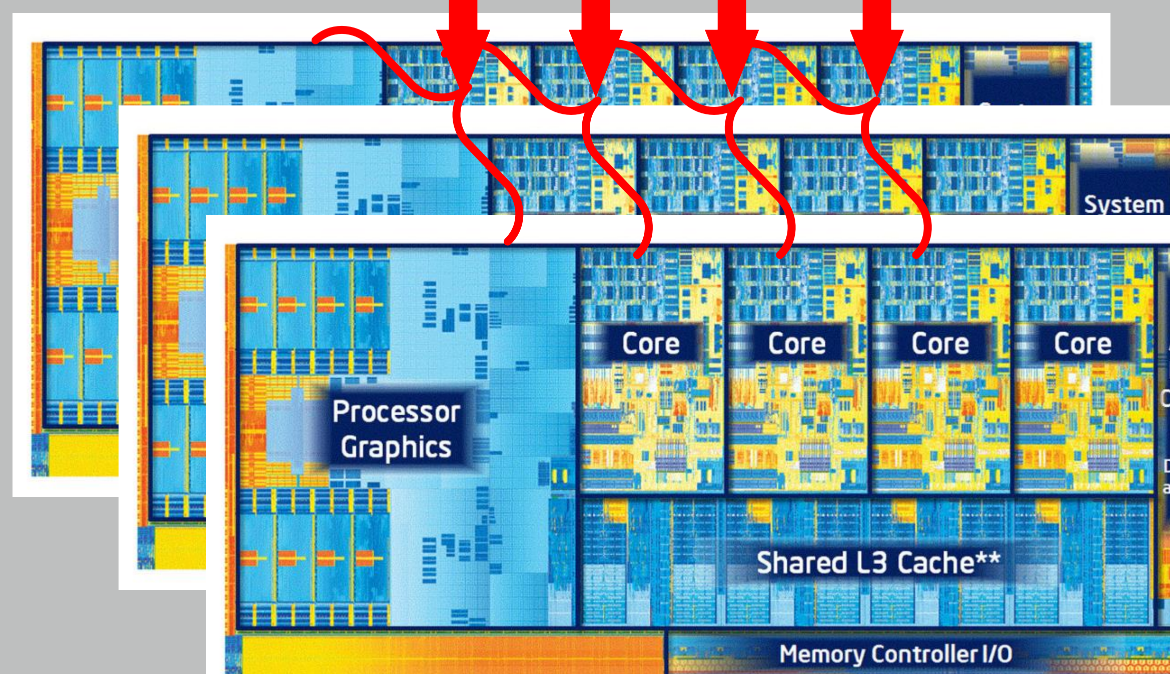
Element loop parallelisation : want more processors ? Use MPI



- Double scale → element intensive model.
- Parallelisation using an OpenMP paradigm.
- Results: speedup up to 9 using a 12 core machine.
- Other approaches: massive parallelization (MPI) **: distributed memory model**

Element loop queue

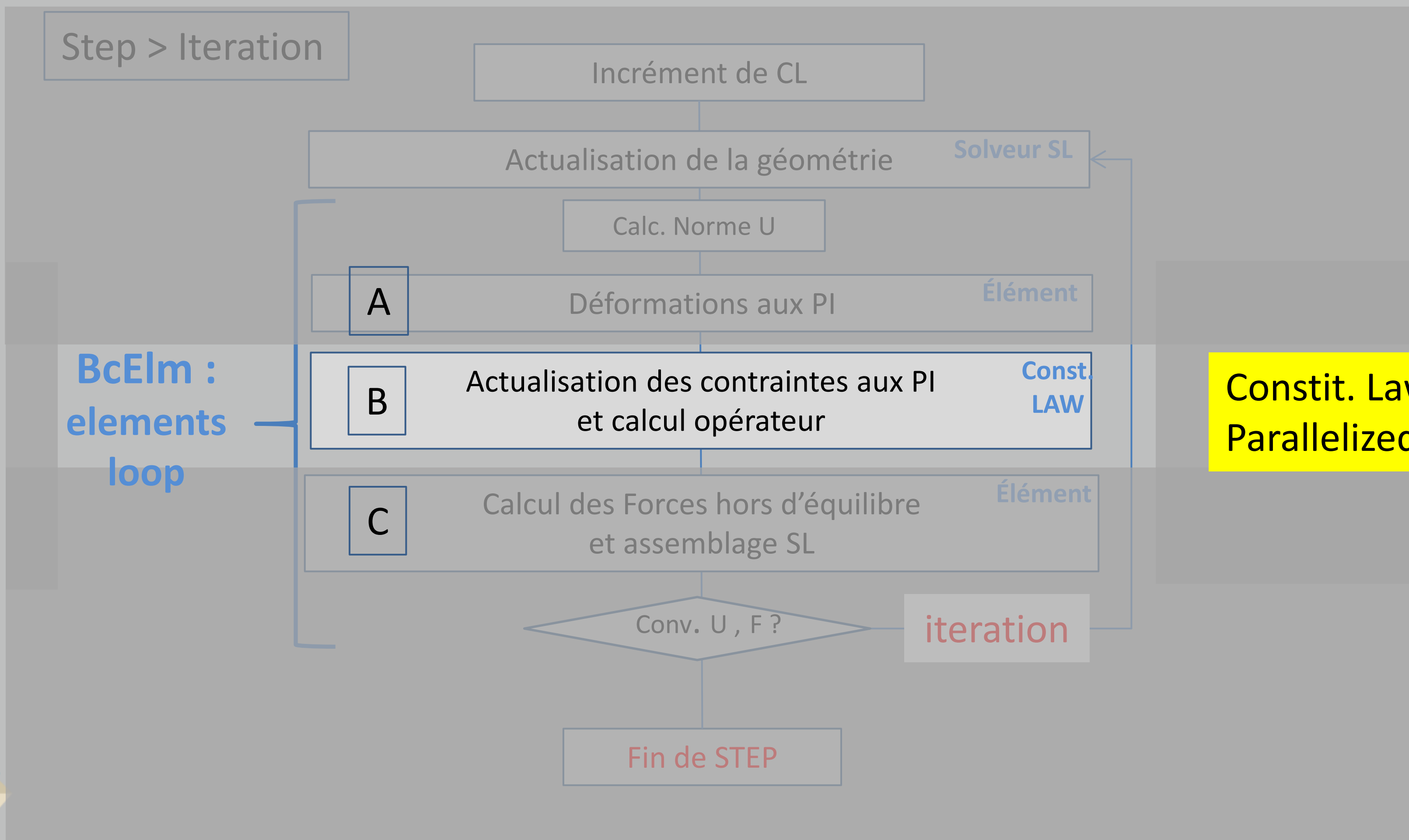
MPI paradigm



Element loop workflow

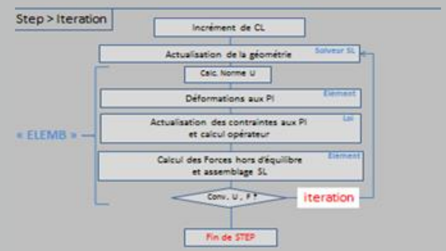
MPI = Message passing Interface

Make a choice : Concentrate on the lower level « atomic » task

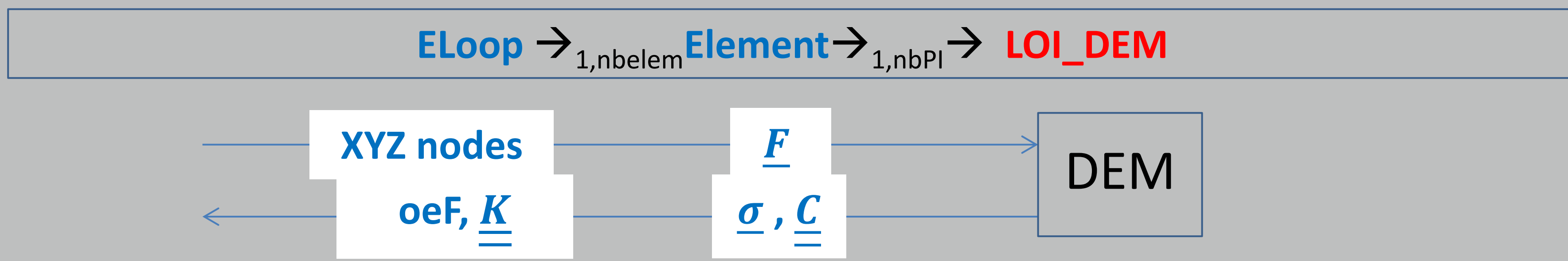


Constit. Law Call Parallelized

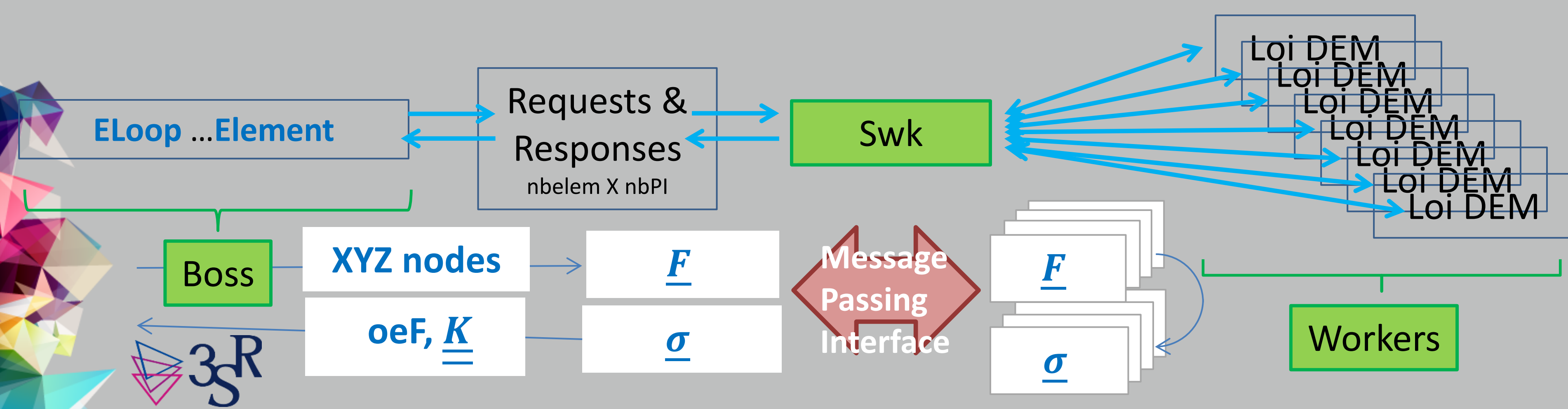
Element loop organisation



- Sequential :



- Parallel MPI with 3 levels: boss, supervisor, wk



Performances
example : Biaxial Test 128 elements with 2nd gradient

- **Sequential REV 400** : step 15 reached in 174 minutes
- **Parallel MPI REV 400**

Nb wks	time	acceler. factor	scalability
1	172'	NA	NA
10	21'	8,2	82%
50	8'	21	43%

- **Sequential REV 1600** : step 15 reached in 3401 minutes
- **Parallel MPI REV 1600** : 77 minutes

Nb wks	time	acceler. factor	scalability
48	77'	37	75%

scability increases with increasing REV size, (for a given number of workers)

→ Scalibility improves with relative « heaviness » of the micro problem

→ Still some acceleration possible with more refined intermediate data recording strategies (experimental, spring 2016, quasi 100% efficiency but increased implementation complexity)

… and a priori no limitation on the number of computers & nodes

3SR

Conclusions & Perspectives

CONCLUSIONS (final)

- We have presented an ***integrated 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)
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PERSPECTIVES

-3D approach (OK spring 2016, still experimental)

-- hydromechanical coupling (idem, ongoing work)

references

Grenoble –Alpes 3SR-Lab team

- [1] Nitka M., Combe G., Dascalu C., Desrues J. Two-scale modeling of granular materials: a DEM-FEM approach, *Granular Matter* vol.13 No 3, pp. 277-281, (2011)
- [2] Nguyen T.K., Combe G., Caillerie D., Desrues J. FEM x DEM modelling of cohesive granular materials: numerical homogenisation and multi-scale simulation, *Acta Geophysica* vol.62 No 5, pp. 1109-1126, (2014)

… more refs to appear shortly

Hong-Kong Univ. team

- [3] Guo Ning and Zhao Jidong. A coupled FEM/DEM approach for hierarchical multiscale modelling of granular media. *International Journal for Numerical Methods in Engineering* 99.11, 789-818 (2014)

… more refs recently appeared