NHL-DEM, a Numerically Homogenized Constitutive Law that works in FEM-DEM multi-scale computations

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Outline

1. Introduction
2. FEM-DEM multiscale modelling : Principle
3. NHL as a constitutive model : ACTIV integration
4. NHL performances (illustrations...)
5. Conclusions & Perspectives

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Multiscale Numerical approach of composite materials : a fast emerging framework

Double-scale approaches : concurrent & collaborating numerical analysis at 2 scales : Macro scale and microscale

- FE^2 (finite element square)
- FEM X DEM
- ...

A very good review paper (2009) :

Arch Comput Methods Eng (2009) 16: 31–75
DOI 10.1007/s11831-008-9028-8

ORIGINAL PAPER

Multiscale Methods for Composites: A Review

P. Kanouté · D.P. Boso · J.L. Chaboche · B.A. Schrefler

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ORIGINAL PAPER

Multiscale Methods fo

P. Kanouté · D.P. Boso · J.L. Chabo

Abstract Various multiscale methods are reviewed in the context of modelling mechanical and thermomechanical responses of composites. They are developed both at the material level and at the structural analysis level, considering sequential or integrated kinds of approaches. More specifically, such schemes like periodic homogenization or mean field approaches are compared and discussed, especially in the context of non linear behaviour. Some recent developments are considered, both in terms of numerical methods (like FE^2) and for more analytical approaches based on Transformation Field Analysis, considering both the homogenization and relocalisation steps in the multiscale methodology. Several examples are shown.

Introduction : bridging scales in Geomechanical 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** ☺ ☺

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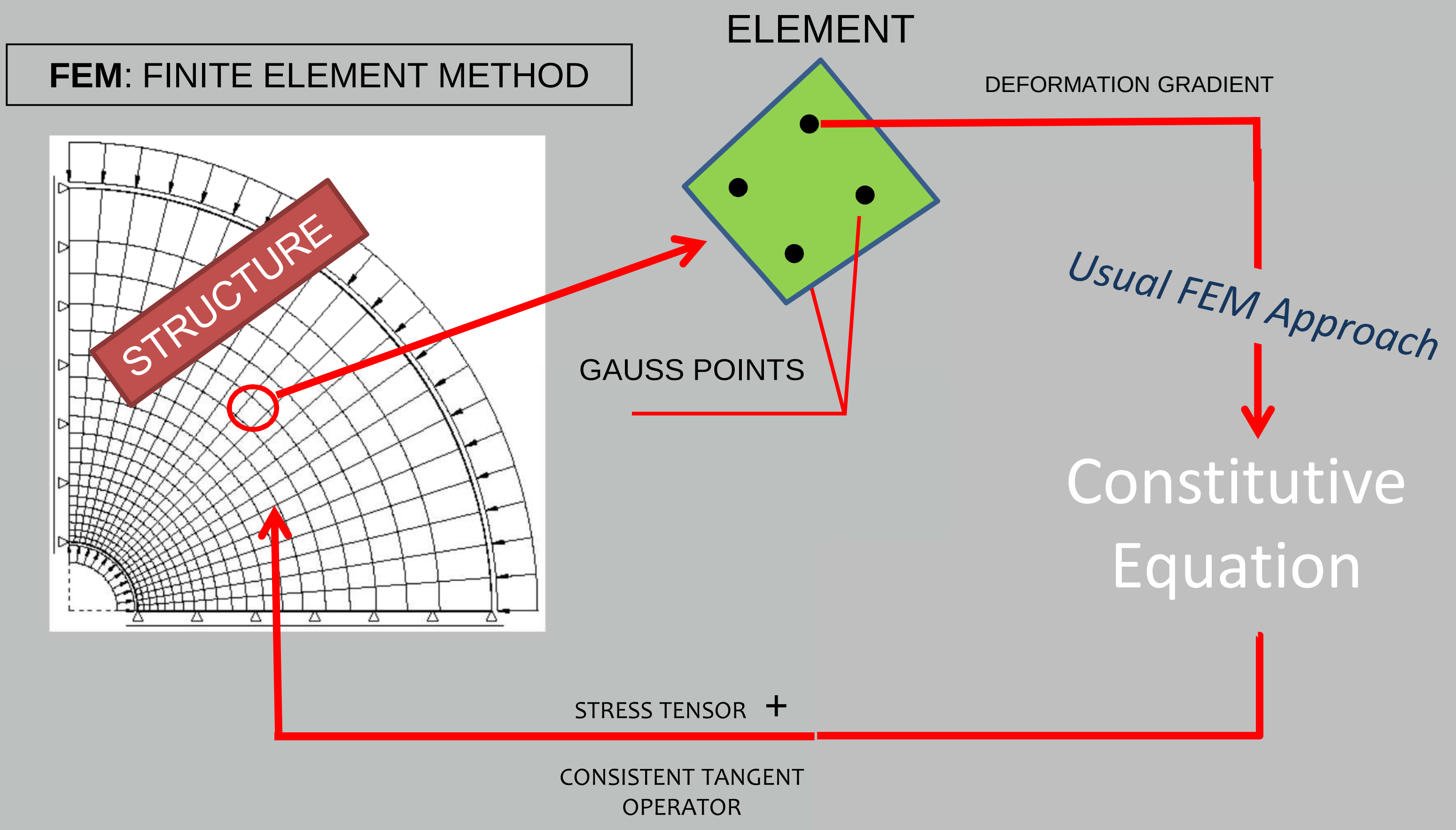
Principle

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



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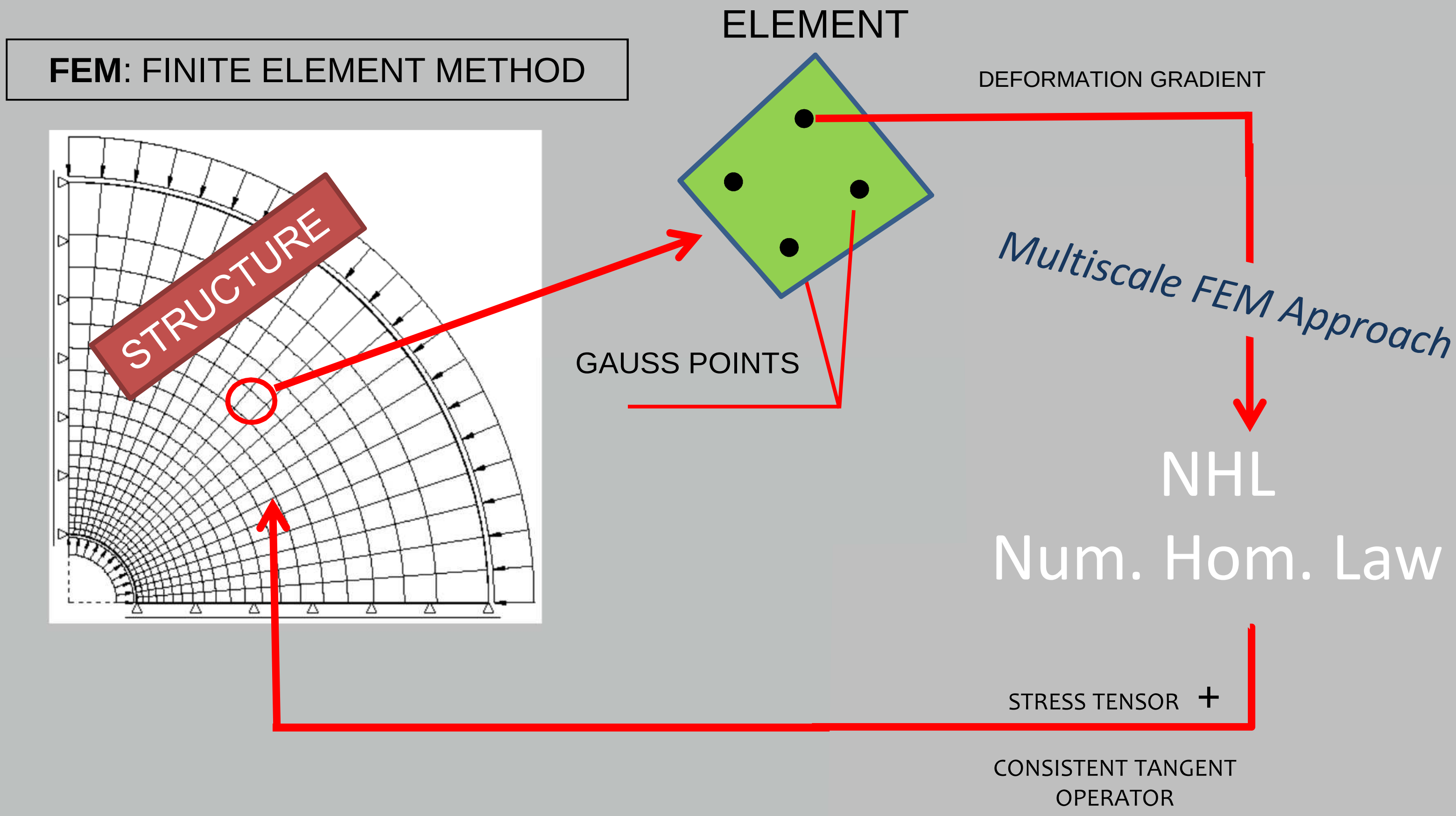
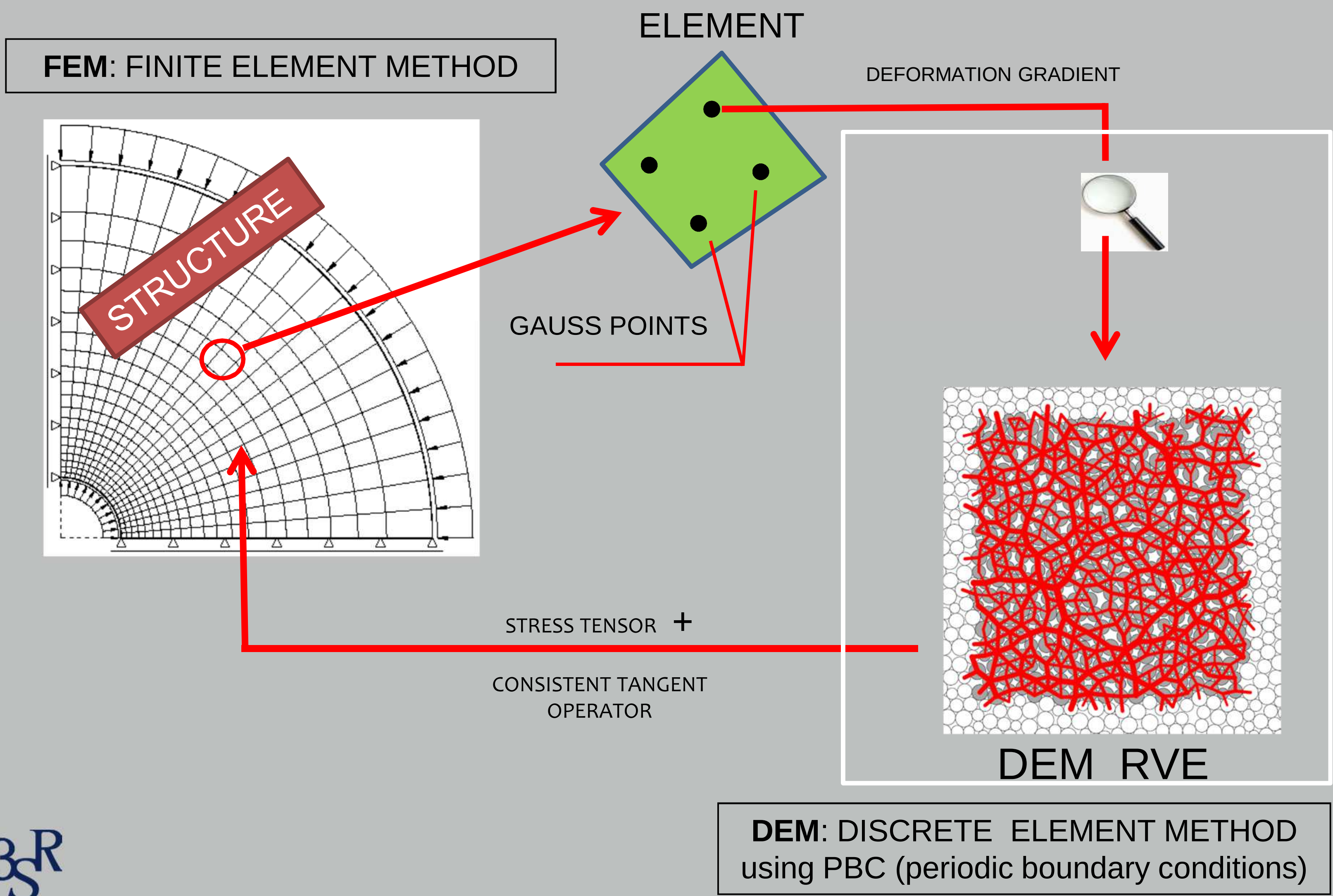
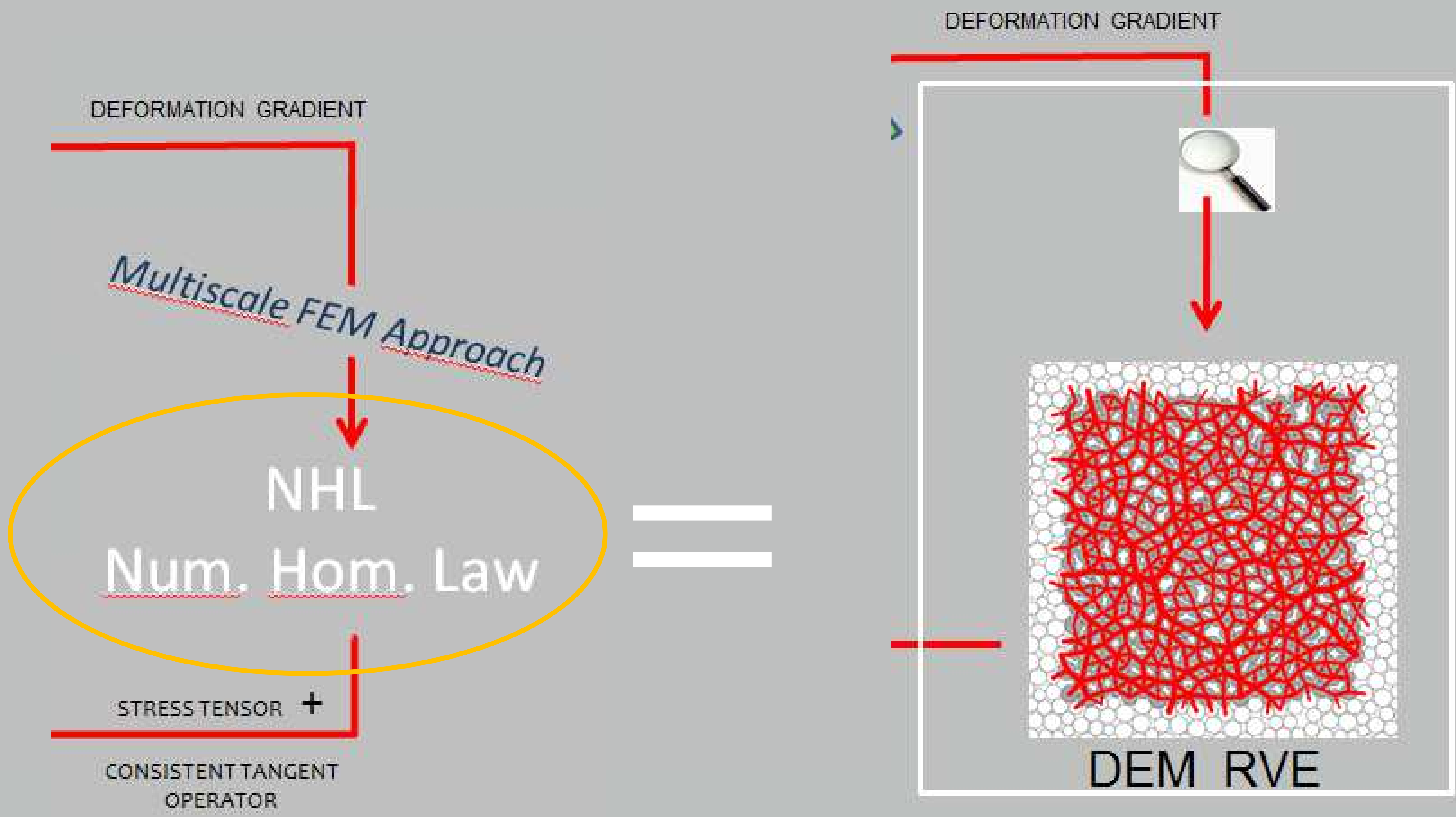


Principle

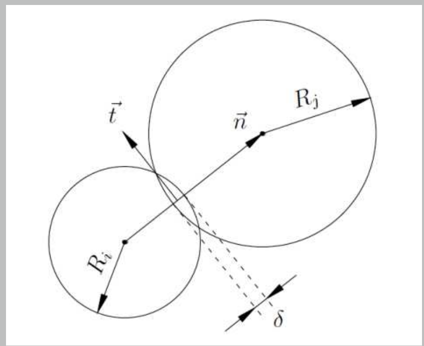
A two-scale numerical homogenization approach by FEM - DEM



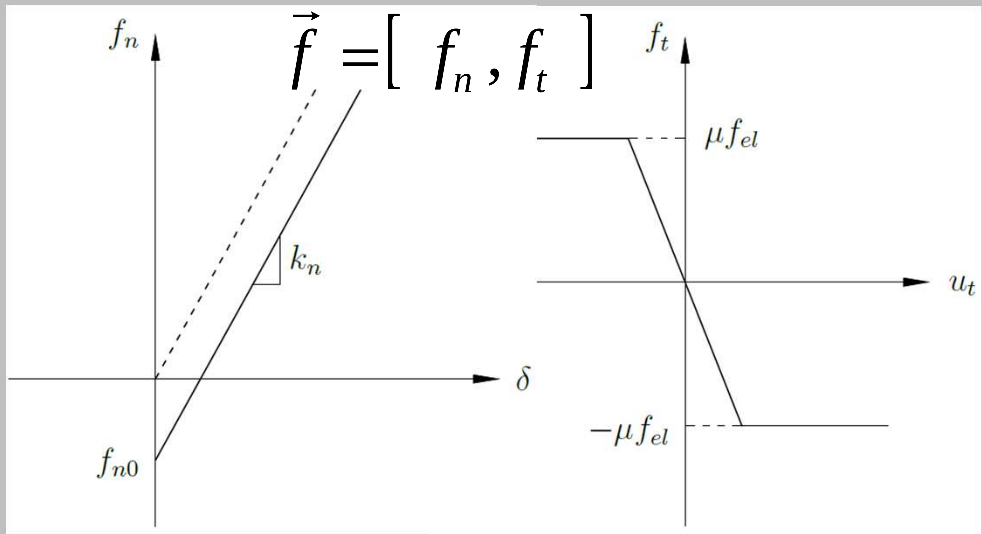
NHL - DEM : DEM-based NHL



Micro-scale Model



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



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

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

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

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

Principle

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

- **FEM code :**
  the choice made has been to use a large multi-purpose FEM code (Lagamine, Liège University Ulg)
- **DEM code** : an as-compact-as-possible DEM kernel
  -> in-house 3SR-Grenoble DEM code, Geochanics team
  strong requirement : quasi-perfect static equilibrium at the end of each DEM step
- **Bridge :**
  direct incorporation of the DEM code as a constituve law in the FEM code (convenient for sequential programming, or OpenMP parallel programming)

Principle

- We develop this framework since 2008

- The other team currently developing FEMxDEM in the world is in Hong-Kong (JiDong Shao, HK University) essentially along the same lines as our work (after our communication in IWBDG 9th in Porquerolles)

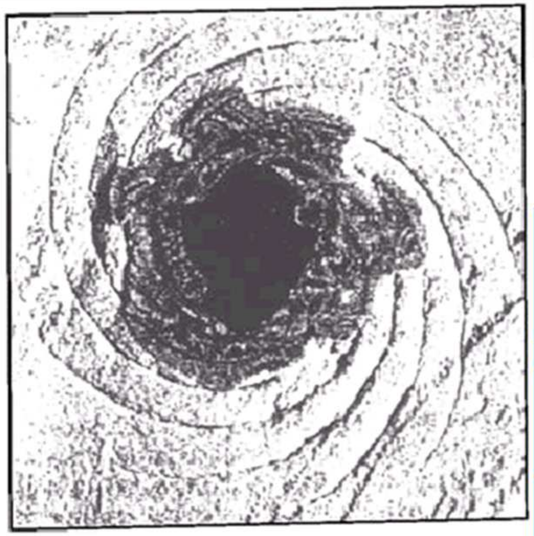
References :
[1] Miehe C, Dettmar J (2004) Comput. Methods Appl. Mech. Engrg, 225-256.
[2] Meier HA, Steinmann P, Kuhl E, Technische Mechanik, Band 28, Heft 1, 2008, 32-42.
[3] Kouznetsova V, Brekelmans WAM, Baaijens FPT (2001) Computational Mechanics 27 37-48.
[4] Nitka M., Combe G., Dascalu C., Desrues J. (2011) Two-scale modeling of granular materials: a DEM-FEM approach, Granular Matter vol.13 No 3, pp. 277-281
[5] Nguyen TK, Combe G, Caillerie D, Desrues J (2013) AIP Conf, Proc. 1542, 1194
[6] Guo, N Zhao, JD (2014) A coupled FEM/DEM approach for hierarchical multiscale modelling of granular media, Int. J. for Numerical Methods in Engineering, Vol.99, No 11, Pages: 789-818
[7] Nguyen, Trung Kien; Combe, Gael; Caillerie, Denis; Desrues, J. (2014) FEM x DEM modelling of cohesive granular materials: Numerical homogenisation and multi-scale simulations, ACTA GEOPHYSICA V.62 No 5 pp: 1109-1126

But first of all, does it really work ?

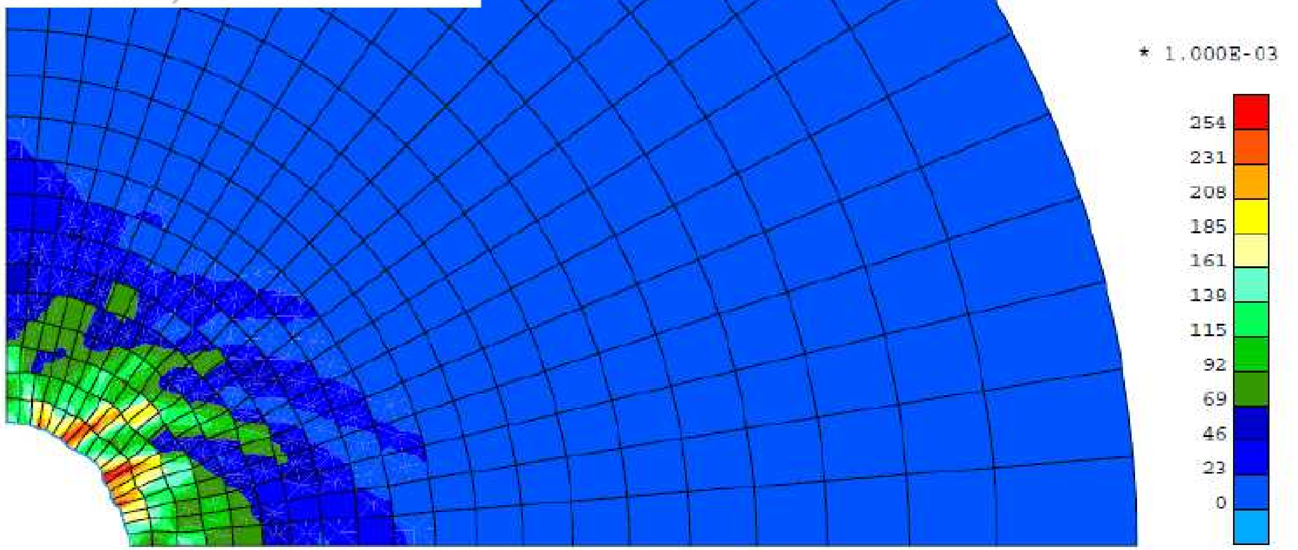
- Too complex …?
- Too CPU demanding …?
- only of academic interest … ?

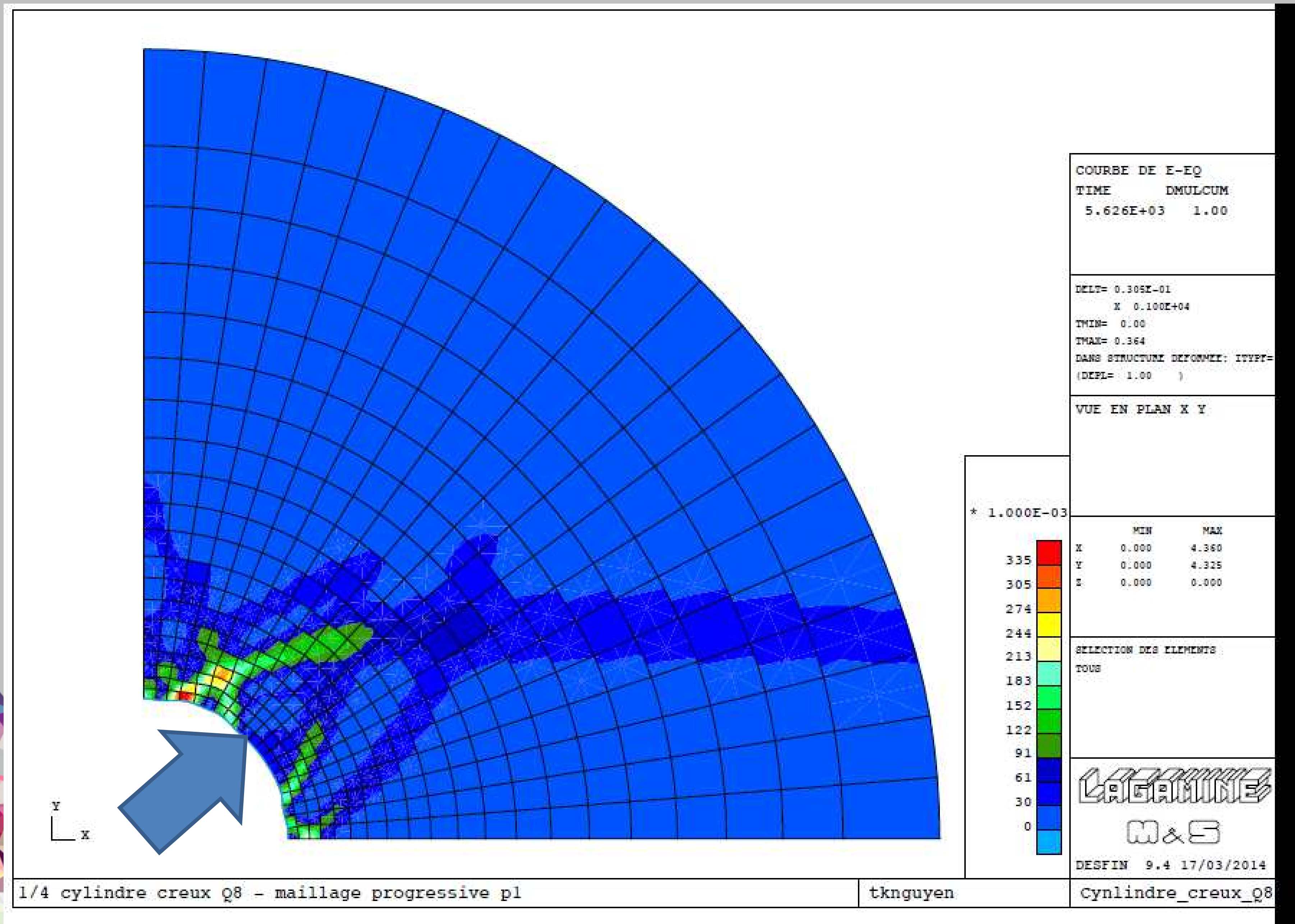
- Just a few examples

Multiscale FEM-DEM Computations



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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1/4 cylindre creux Q8 - maillage progressive p1
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NHL-DEM as a constitutive model

- **NHL** ***is*** a constitutive model in the general form : $\boldsymbol{F}_{\tau \leq t} \rightarrow \boldsymbol{\sigma}_{\tau \leq t}$

with $\boldsymbol{a}_{\tau \leq t}$ history of the function $\boldsymbol{a}$ i.e. $\boldsymbol{a}_{\tau \leq t} = \{\boldsymbol{a}(\boldsymbol{\tau}), \boldsymbol{\tau} \in [\mathbf{0}, \boldsymbol{t}]\}$

Building the constitutive law $\boldsymbol{F}_{\tau \leq t} \rightarrow \boldsymbol{\sigma}_{\tau \leq t}$ is an evolution problem

- **NHL** is built using a ***step by step*** method which rely on the numerical homogenisation of a RVE modelled using DEM : $\boldsymbol{F}^n \rightarrow \boldsymbol{\sigma}^n$

If $\boldsymbol{F}^n$ and $\boldsymbol{\sigma}^n$ are the values of $\boldsymbol{F}$ and $\boldsymbol{\sigma}$ at the end of the step $\boldsymbol{n}$, then we write :

$$\boldsymbol{\sigma}^n = \boldsymbol{\Sigma}^n(\boldsymbol{F}^n)$$

assuming that $\boldsymbol{\Sigma}^n$ is differentiable we write :

$$\boldsymbol{\delta\sigma}^n = \boldsymbol{\Sigma}^n(\boldsymbol{F}^n + \boldsymbol{\delta F}^n) - \boldsymbol{\Sigma}^n(\boldsymbol{F}^n) = \boldsymbol{C}^n : \boldsymbol{\delta F}^n + \cdots$$

with $\boldsymbol{C}^n$ a four rank tensor : $\boldsymbol{C}^n = \dfrac{\boldsymbol{d\Sigma}^n}{\boldsymbol{dF}^n}$

NHL-DEM as a constitutive model - I/II

- The numerical homogenisation approach to constitutive modelling offers **specific and remarkable performances** with respect to **difficult-to-model material behaviours :**

- / strain-softening / inherent and induced anisotropy / principal stress rotation / cyclic response / compression-extension cycles / …

- All these performances results simply from the fact that the **state** of the material (i.e. the RVE) is **exhaustively** described by the set of (state) variables which are :

  the position of the grains, the ***actual list of contacts*** AND the ***forces*** at these contacts

- Next : ACTIV

NHL-DEM as a constitutive model - II/II

- To perform the exploration of such constitutive responses,
  a ***material-point*** constitutive integration code "ACTIV" is used,

- ACTIV is an *in-house* 3SR-Grenoble development, initially created with the hypoplastic CLoE model in the years 1990' (both still in use).

- ACTIV allows to impose
  any combination of stress and strain components to an elementary volume and compute the constitutive response to this loading program
  i.e. the *complementary stress and strain components*

Examples :
Triaxial test : starting from an initial stress state (consistent with the RVE intergranular forces),
i) isotropic loading to a given stress state, then ii) deviatoric loading, either strain-controlled or stress controlled.
Cyclic triaxial test, either stress or strain controlled

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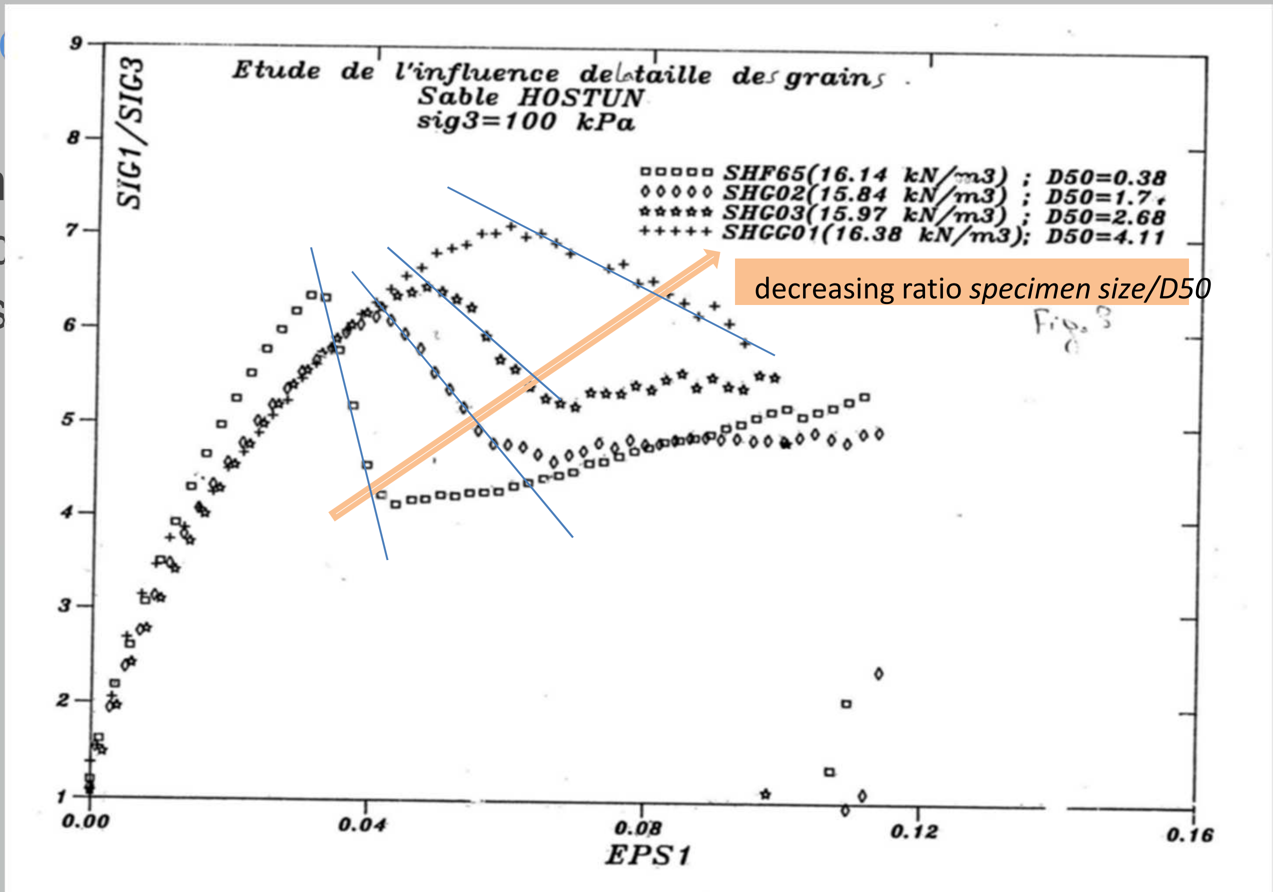
NHL-DEM performances :

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

NHL-DEM performances :

strain softening and strain localisation

- Strength reduction of specimens in laboratory tests : a structural response or a material response ? Extremely difficult to assess experimentally
  - e.g., scale dependency in the test response : due to localisation, smaller specimens show smaller strain softening rate
- Then, intr… …al basis
- DEM com… …olution of contacts c… …tion (void ratio), des…



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- Then, introducting strain softening in phenomenological constitutive laws is lacking a sound experimental basis
- DEM computations provide strain softening on a micro-structural basis : evolution of contacts distribution and orientation, grain rotation, changes in grain distribution (void ratio), destruction of cohesive links

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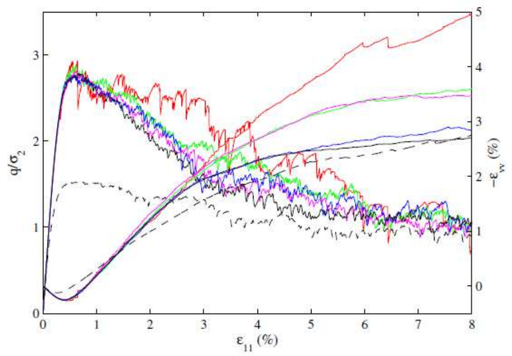

FIGURE 2.18 – Réponses macroscopiques des essais biaxiaux en compression : VER400 (rouge), VER3600 (vert), VER6400 (rose), VER10000 (bleu) et VER22500 (noir). La réponse en noir pointillé est celle du cas sans cohésion du VER10000, avec : $\kappa = k_n/(\sigma_0 \cdot \bar{a}) = 1000$, $k_n/k_t = 1$, $\mu = 0.5$ et $p^* = 0$.

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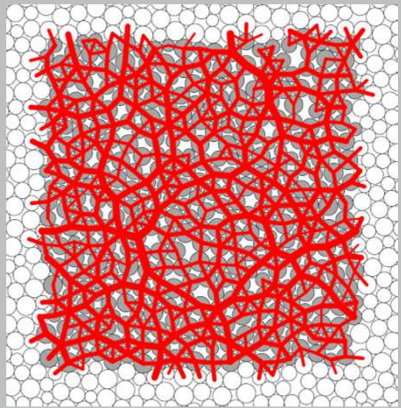
Strain softening : Micro-scale Model response

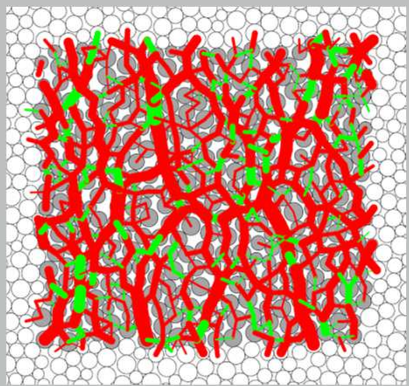
Biaxial test (DEM with PBC): REV contains 400 particles



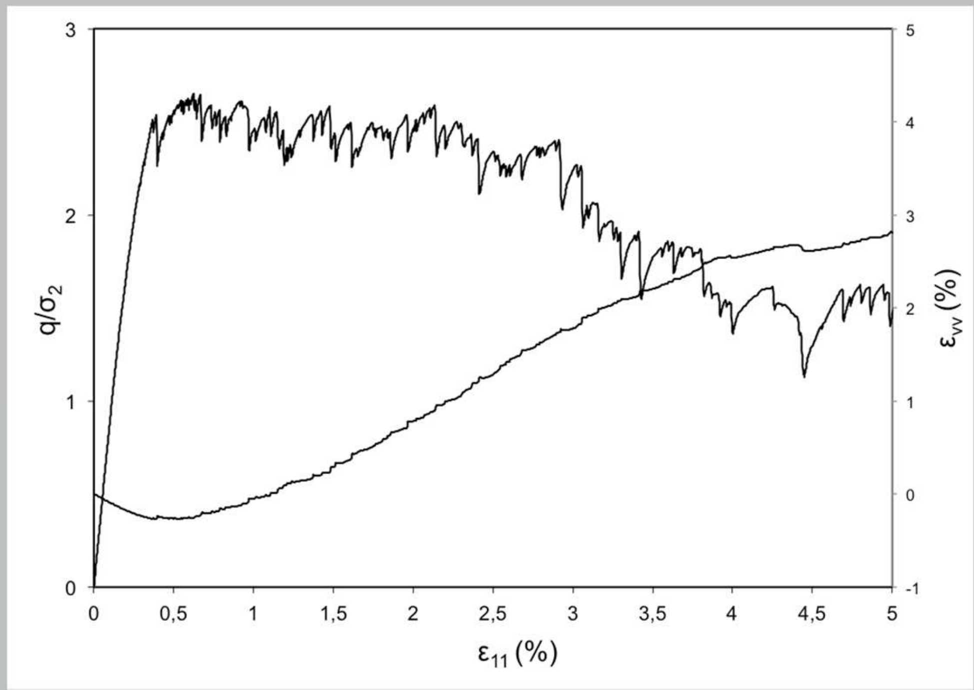
Initial configuration

— f_c effective

— $f_c = 0$

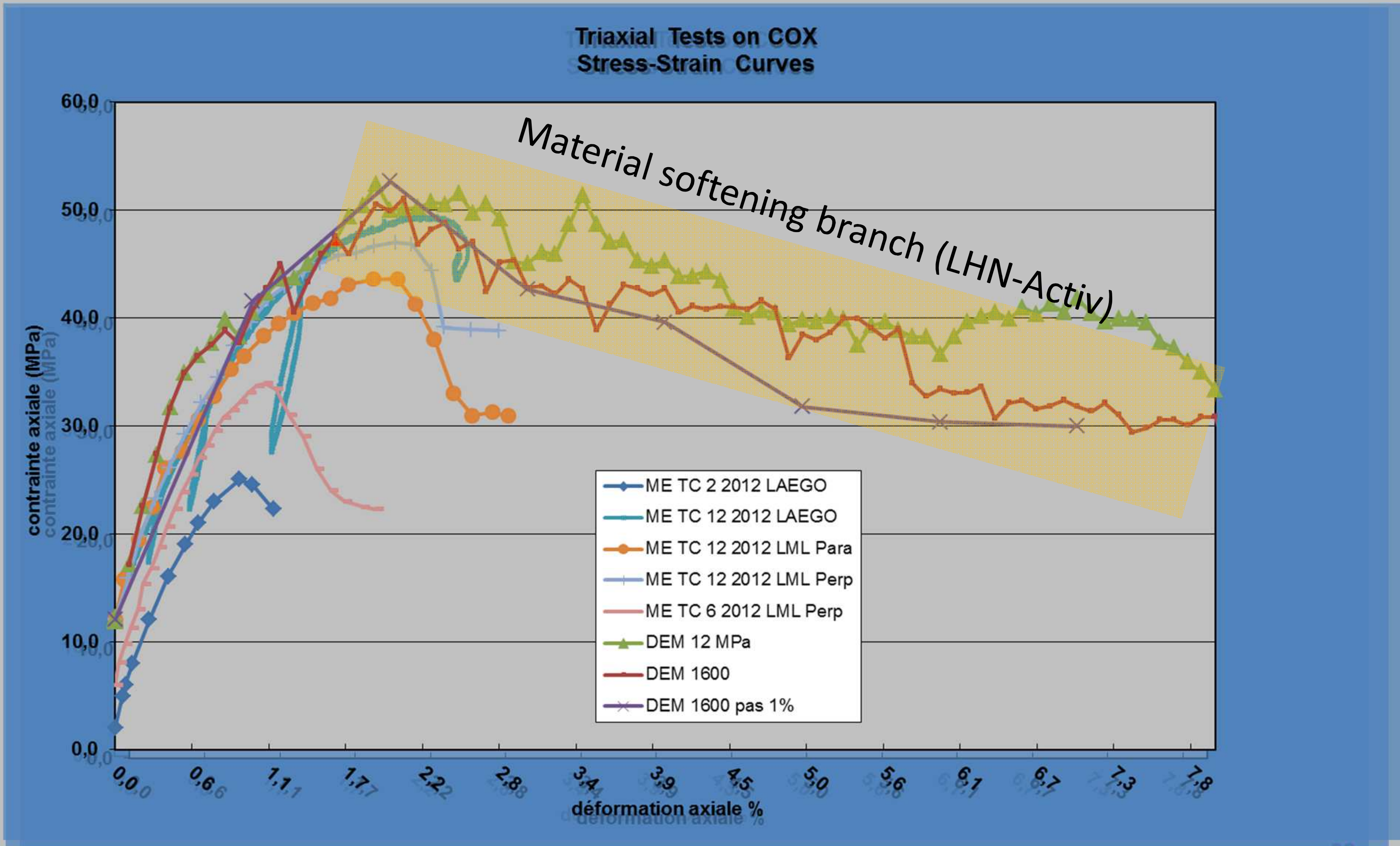


at 3% of axial strain (ε_{11})

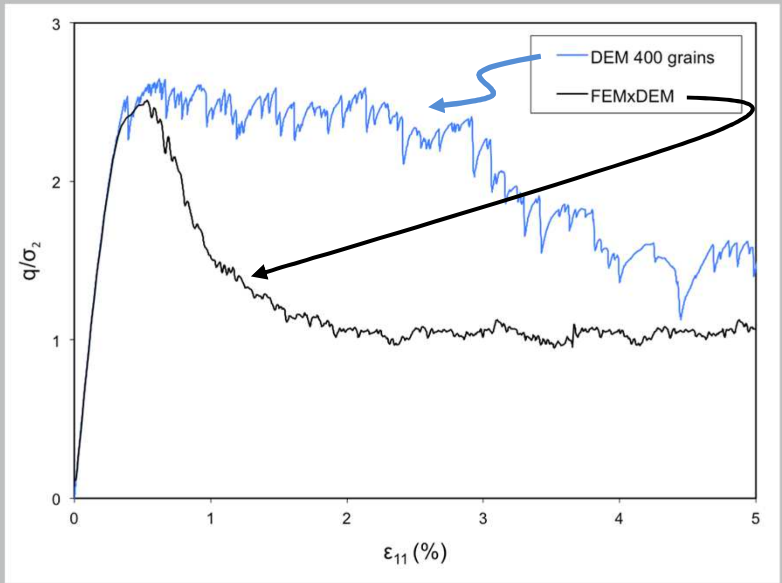


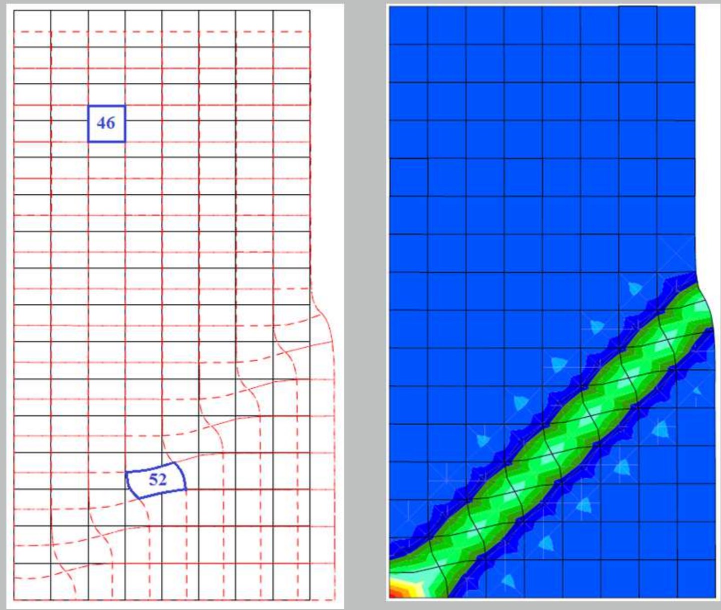
Strain Softening : LHN response (via Activ)

Triaxial test on a cohesive geomaterial

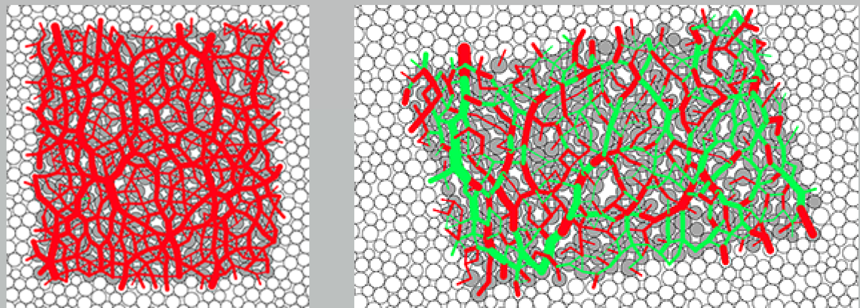


Strain Softening and Strain localization : FEM x DEM response





Deformed structure and second invariant of strain tensor



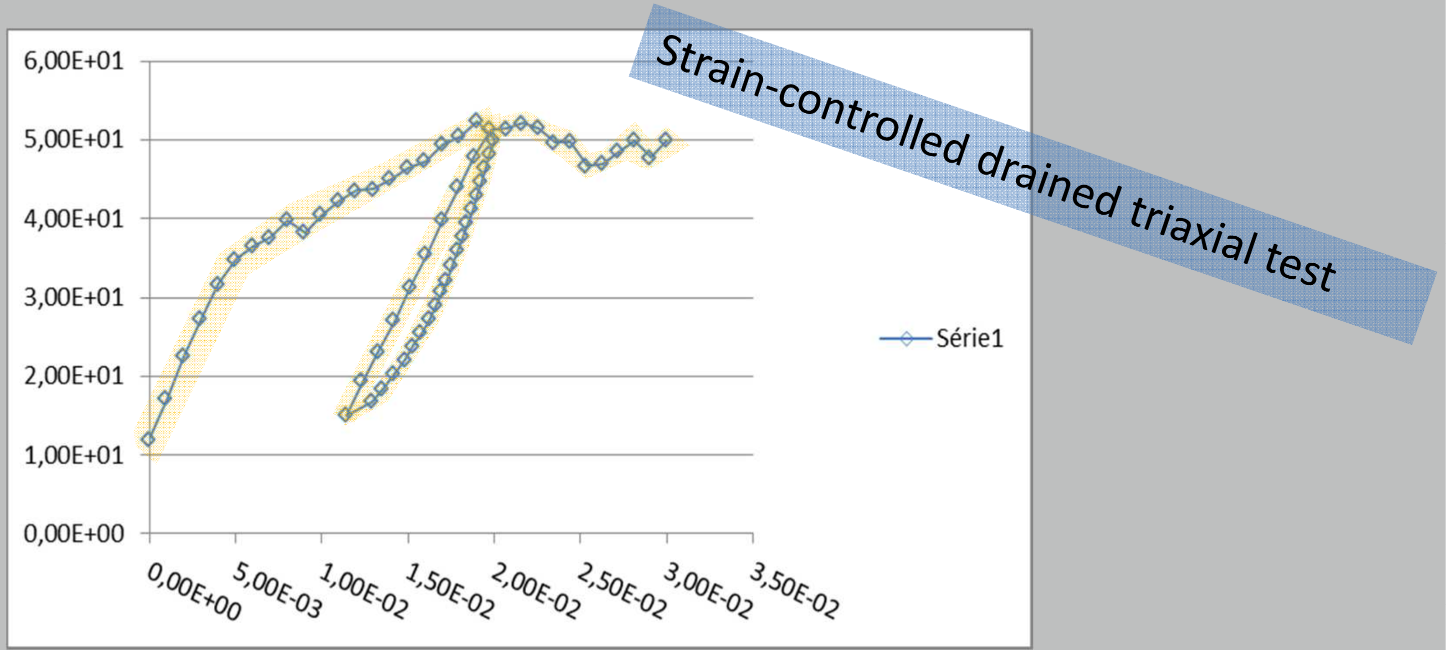
Element 46 Element 52

Deformed REV

NHL-DEM performances :

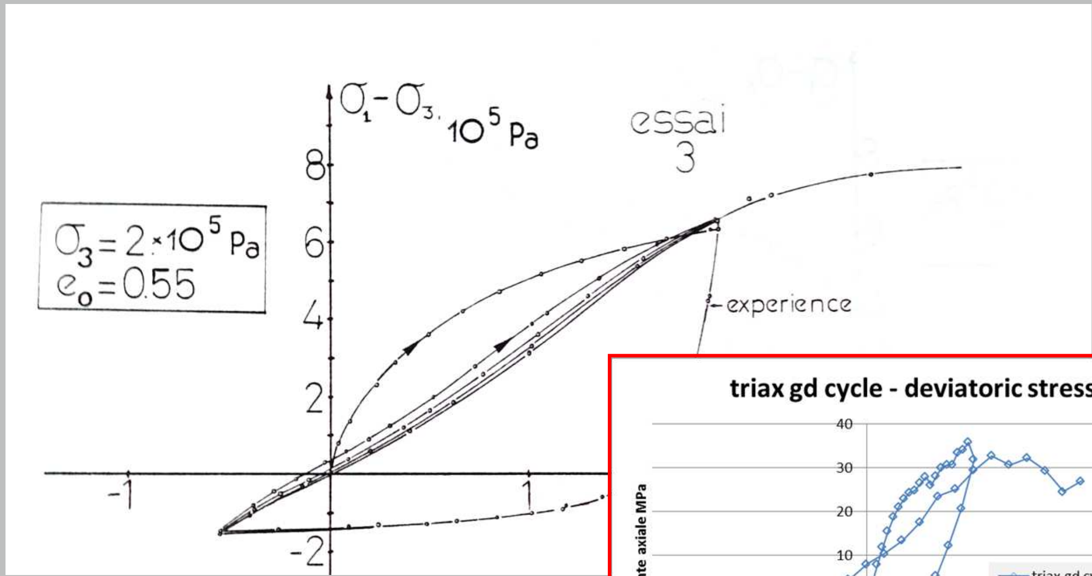
- Strain softening and strain localisation
- Cyclic response
- Anisotropy
- Principal stress rotations

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



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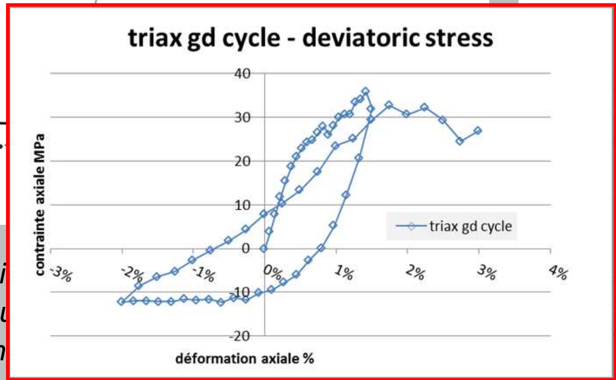

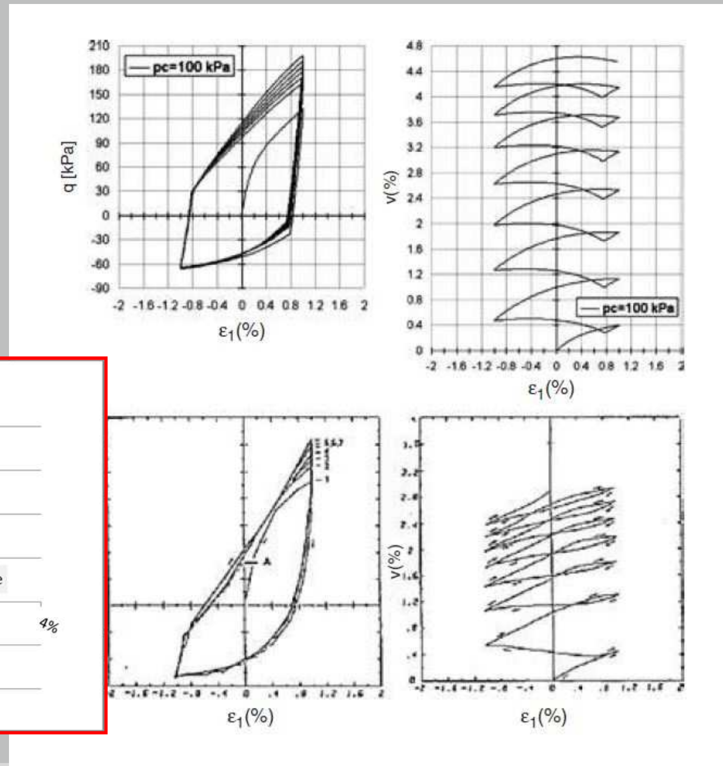

Figure 4. Drained cyclic compression/extension test on medium loose Hostun RF sand: (a) numerical simulations, (b) experimental data (Mohkam 1983).

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

*C. Zambelli, C. di Prisco & S. Imposimato (2004) **A cyclic elasto-viscoplastic constitutive model:** theoretical discussion and validation, in Cyclic Behaviour of Soils and Liquefaction Phenomena, Triantafyllidis (ed)© 2004 Taylor & Francis Group, London*

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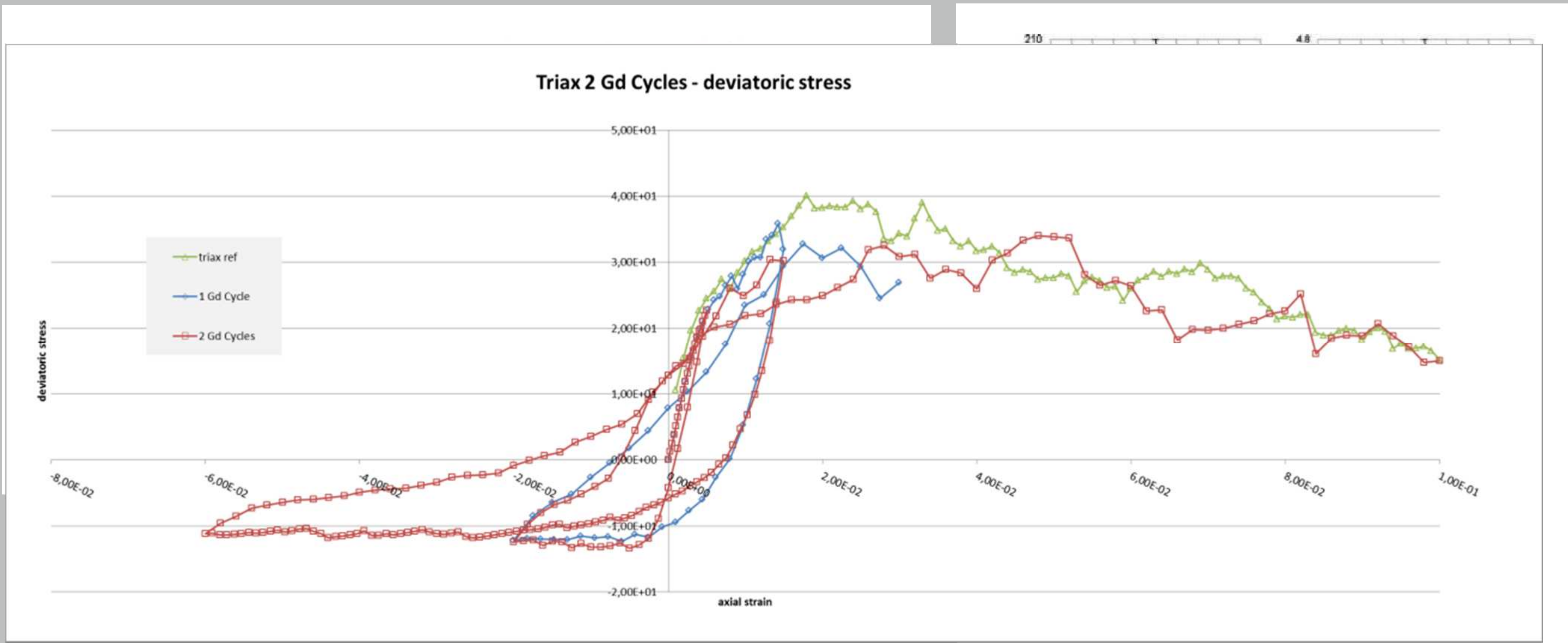
NHL-DEM performances :
triaxial compression-extension cycles



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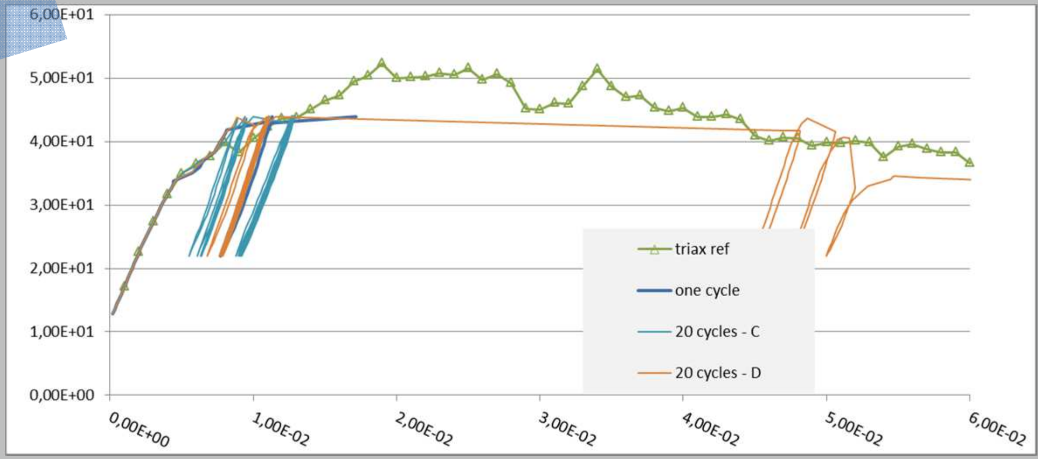
NHL-DEM performances : multi-cycles

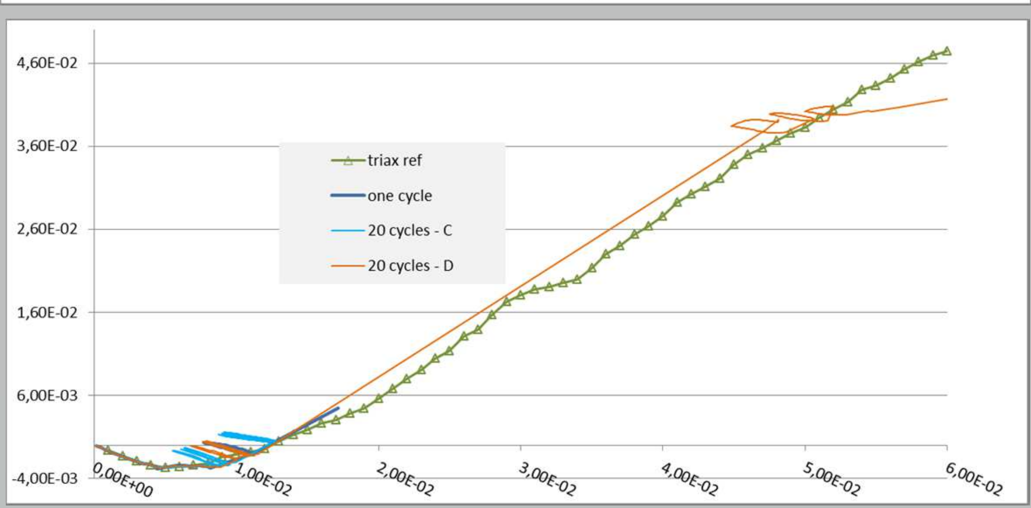
STRESS-controlled drained triaxial test

Loading program : 20 cycles , axial stress [20-40] Mpa
Each cycle is performed in 20 steps, except the 1st one (40 steps)

12.0	44.0	12.00	0.0	40	0000
12.0	22.0	12.00	0.0	20	0000
12.0	44.0	12.00	0.0	20	0000
12.0	22.0	12.00	0.0	20	0000
12.0	44.0	12.00	0.0	20	0000
12.0	22.0	12.00	0.0	20	0000
12.0	44.0	12.00	0.0	20	0000
12.0	22.0	12.00	0.0	20	0000
12.0	44.0	12.00	0.0	20	0000
12.0	22.0	12.00	0.0	20	0000
12.0	44.0	12.00	0.0	20	0000
12.0	22.0	12.00	0.0	20	0000
12.0	44.0	12.00	0.0	20	0000
12.0	22.0	12.00	0.0	20	0000
12.0	44.0	12.00	0.0	20	0000
12.0	22.0	12.00	0.0	20	0000
12.0	44.0	12.00	0.0	20	0000
12.0	22.0	12.00	0.0	20	0000
12.0	44.0	12.00	0.0	20	0000
12.0	22.0	12.00	0.0	20	0000

Reference triaxial : strain controlled, up to axial strain = 10%

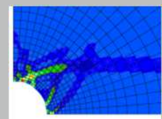




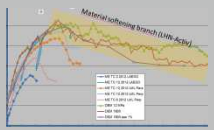
Conclusions & Perspectives

CONCLUSIONS

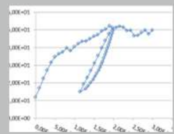
- We have presented a Two-scale numerical approach for granular materials: combining FEM (at macro scale) and DEM (at micro scale).
- Illustration by 2 examples of BVP on a hollow cylinder analogous to i) underground excavations and drilling, or ii) cavity expansion.



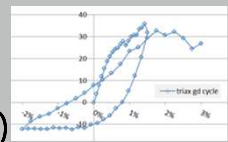
-Focusing on the constitutive law NHL-DEM = numerically homogenised law based on the micro-scale DEM simulation, we have studied the response of the law to simple and complex stress-strain paths :



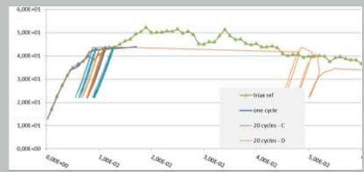
- Strain softening on triaxial path -> localisation in FEM



- Cyclic response (one cycle, small)
- Cyclic response (one or two large cycles, with compression-extension)



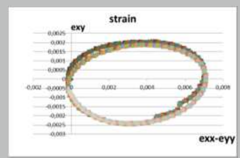
- Multi cyclic response with temporary loss of control



NOT PRESENTED

principal stress rotation

anisotropy



PERSPECTIVES

- Second gradient regularisation

-Parallelisation (massive preferably)

-3D approach

Thank you for your attention

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