Non Smooth Approaches for the simulation of divided media

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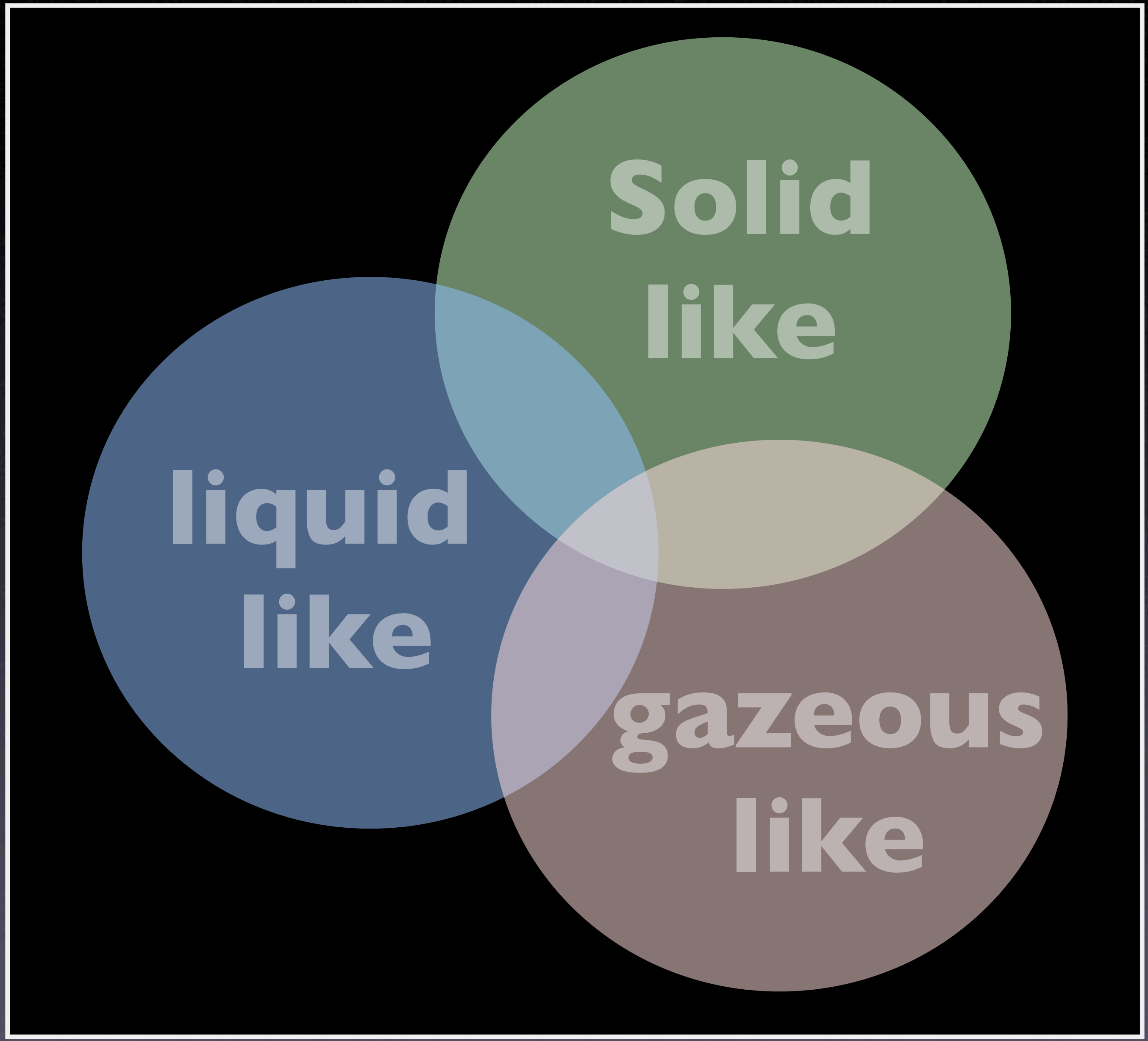


The well known *Granular Tryptic*

Around us, numerous media presents naturally a divided feature:
granular material, masonries, steel at the microstructure level, geophysical structure

Other media present this feature locally under evolutive process such as:
wear, fracture, fissuration,...

For both kind of systems, continuous mechanics cannot be applied, and it become necessary to use more appropriate tools to deal with this discontinuous feature.

Geophysics *Fault and Fold propagation*

In some geophysical applications, hypothesis of continuous mechanics are not available. This is typical the case of Forced Fold evolution and fault propagation.

Fault propagation leads to fracture process and separation

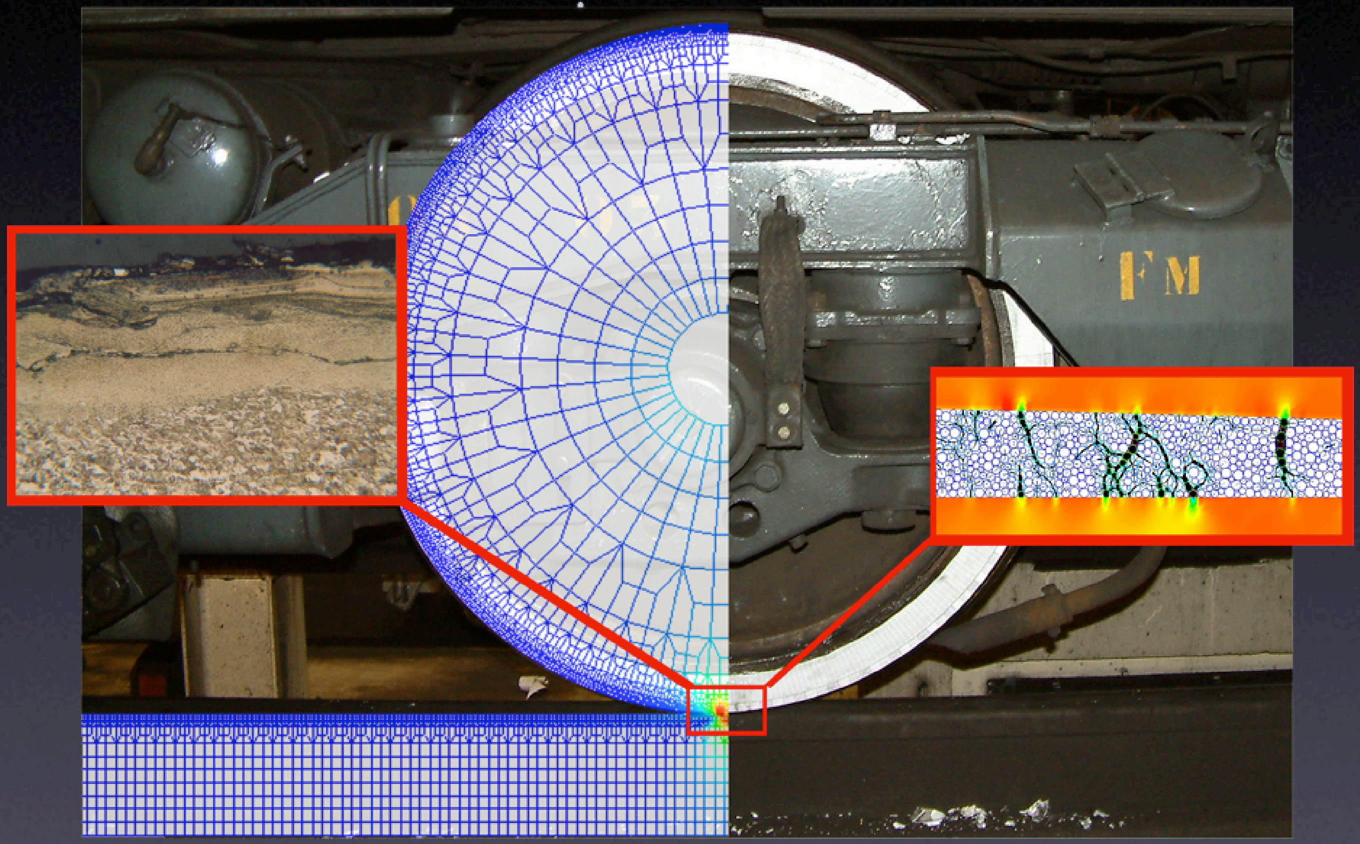
Forced fold evolution leads to fracture process, mixing and surface flow

Analogic sandbox used for experiments

Examples of DEM in geophysics

[1] Burbridge and Braun (2002), *Geophys. J. Int.,* **vol.** 148, p542-561.
[2] Finch et al (2003), *J. Struct. Geol.*, **vol.** 25, pp 515-528.
[3] Hardy and Finch (2006), *Tectonophysics*, **vol.** 415, pp 225-238.
[4] Renouf et al (2006), *Rev. Euro. Meth. Num.,* **vol.** 15 pp. 549-570.
[5] Taboada et al (2005) *J. Geoph. Research*, **vol.** 110, p. B09202.

Tribology ***third-body rheology***



Multi-scale and multiphysic feature of wheel-rail contact: influence of the rheology of the interface (third-body) on the behaviour of the bodies in contact - *the butterfly effect.*

Examples in Tribology

[1] Fillot et al (2005), ASME J. Tribology.
[2] Renouf et al (2006), ECCOMAS 2006.
[3] Renouf et al (2007) Int. J. Num. Method. Engrg.
[4] Seve et al (2002), *ASME J. Tribology*.

1 ***Non Smooth Contact Dynamics***

Overview of the original framework

2 ***Algorithm development***

NSCD optimization

3 ***Simulation results***

Mechanics, Geophysics, Virtual Reality, Tribology ...

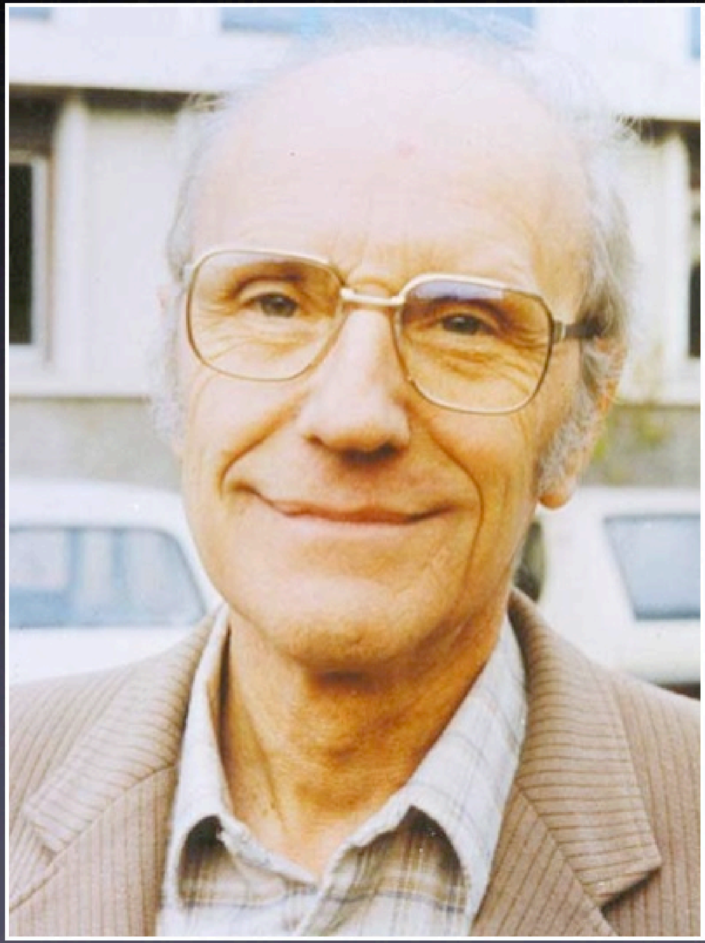
4 ***Conclusions***

What about the future of divided media !

Non Smooth Contact Dynamics

Overview of the original framework

1. *A brief history*
2. *From global frame to local one*
3. *Contact problem resolution*
4. *Contact law panel*



J.-J. Moreau (1983)

1. A brief history (1/2)

In 1994, *J.-J. Moreau* proposed a **non smooth** alternative of the method developped by Cundall for the simulation of multi-contact systems*.

The non smooth feature of the approach is threefold:

**** a non smoothness in space***

limitation of the set of admissible configurations due to the unilateral constraint

**** a non smoothness in time***

discontinuity of velocity due to collisions

**** a non smoothness in force-law***

irregular relationships between forces and configuration

*multi-contact system: systems where the number of contacts is larger than the number of bodies

1. A brief history (2/2)

The non smooth feature involved in the simulation of multi-contact assemblies are aborded in the sense of the Nonsmooth Mechanics (Moreau 1988), a systematization of Convex Analysis and Multivalued Analyis.

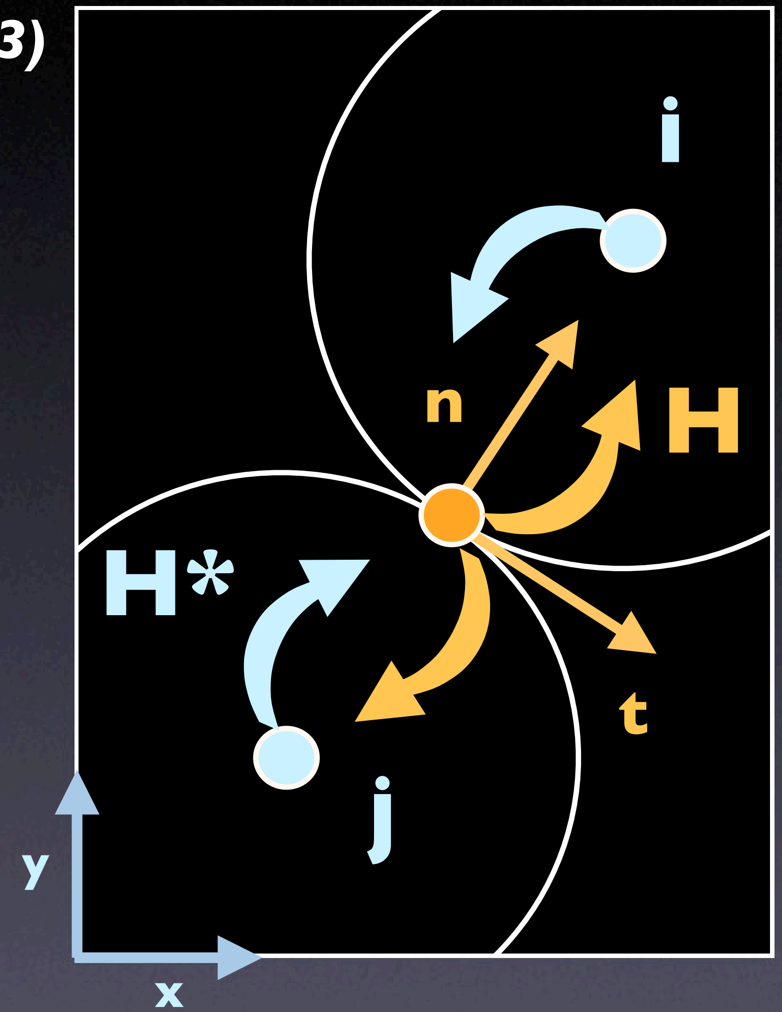
This approach, which allows the treatment of collision and lasting contacts during the same time-step, is called Contact Dynamics (CD).

The generalisation of CD to the simulation of the assembly of deformable bodies is proposed by M. Jean in 1994, under the name *Non Smooth Contact Dynamics*

References:

[1] J.-J Moreau et al, *Topics in Nonsmooth mechanics*, 1988
[2] J.-J. Moreau, *Eur. J. Mech. A/Solids*, **vol.** 13 n° 4 - suppl. pp. 93-114, 1994
[3] M. Jean,
[4] M. Jean, *Comput. Methods Appl. Mech. Engrg*, **vol.** 177, pp 225-237, 1999

2. *From global frame to local one (1/3)*



In the simulation of divided-media, two levels must be considered:

* **the global level** related to **bodies** configuration in the global frame

* **the local level** related to **contacts** variables expressed in each frame

The system

$$\begin{cases} \mathbf{R} = \mathbb{H} r \\ \mathbf{v} = \mathbb{H}^* \mathbf{q} \end{cases}$$

allows the transfert of information between the two levels usinsg the two linear mapping **H** and **H***

2. From global frame to local one (2/3)

As in multi-contact assemblies, many shocks are expected (involving velocity discontinuity), the second time derivative of the configuration parameter cannot be defined.

Thus the classical equation of motion

$$\mathbb{M}\ddot{\mathbf{q}} = \mathbf{F}_{ext}(t, \mathbf{q}, \dot{\mathbf{q}}) + \mathbf{R} \qquad [1]$$

must be reformulated in terms of a measure differential equation,

$$\mathbb{M}d\dot{\mathbf{q}} = \mathbf{F}_{ext}(t, \mathbf{q}, \dot{\mathbf{q}})dt + d\mathbf{R} \qquad [2]$$

where *dt* is the Lebesgue measure on the space of real **R**, d**q** is a differential measure representing the acceleration measure and d**R** is a non-negative real measure.

2. From global frame to local one (3/3)

Over the time interval $[t_i,t_{i+1}[$, the equation [2] is discretized using a θ-method and written in the local frames associated to the set of contacts.

Using the previous linear mapping, the resulting equation is

$$\mathbb{W}h\mathbf{r}_{i+1} - \mathbf{v}_{i+1} = -\mathbf{v}_{free} \qquad [3]$$

where $\mathbb{W}$ is called Delassus operator (= $\mathbb{H}^*\mathbb{M}^{-1}\mathbb{H}$).

To obtain a solution of equation [3], contact conditions are expressed through a contact law, leading to the well known contact problem

$$\left\{ \begin{array}{l} \mathbb{W}h\mathbf{r}(i+1) - \mathbf{v}(i+1) = -\mathbf{v}_{free} \\ ContactLaw(\mathbf{r}(i+1), \mathbf{v}(i+1)) \end{array} \right. \qquad [4]$$

3. Contact law (1/2)

Frictionless contact law: the Signorini condition

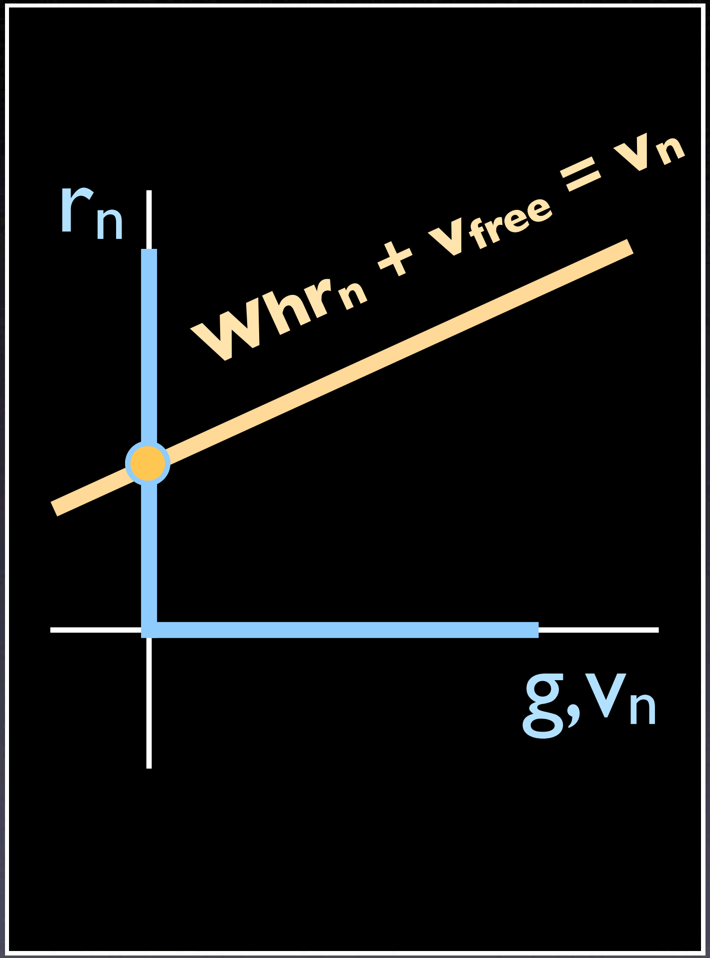
$$r_n \geq 0 \quad g \geq 0 \quad r_n.g = 0 \qquad [5]$$

With the condition

$$\exists t_0 \in [t_i, t_{i+1}[\quad | \quad g(t_0) < 0$$

the relations [5] are equivalent to the well known *velocity Signorini condition*

$$r_n \geq 0 \quad v_n \geq 0 \quad r_n.v_n = 0 \qquad [6]$$



3. Contact law (2/2)

The previous unilateral condition can be completed by:

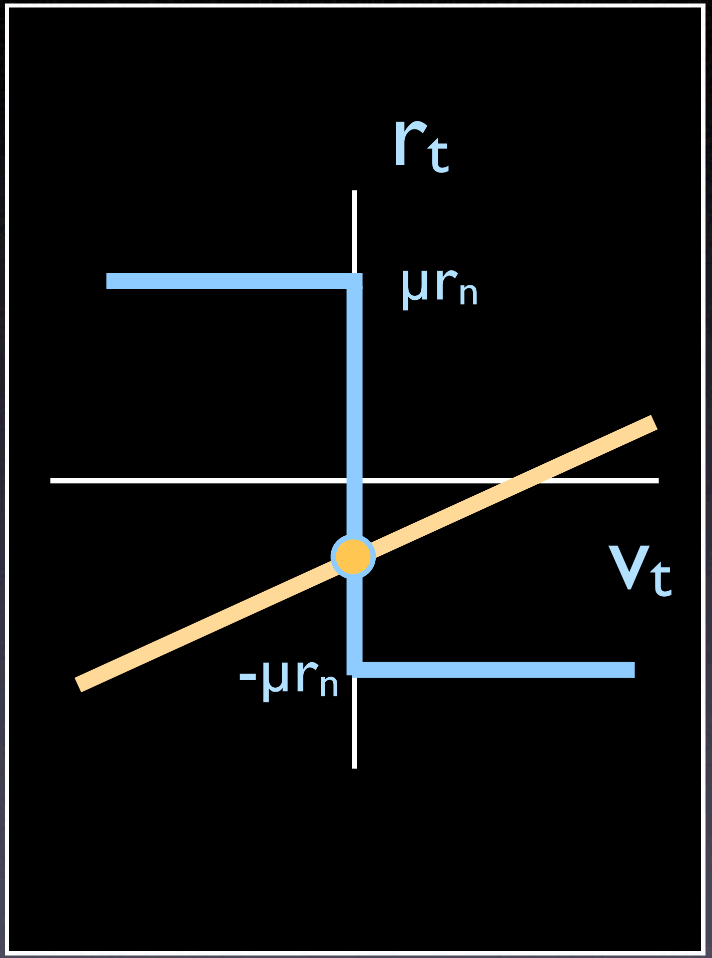
* the classical *Coulomb friction law*

$$\begin{array}{llll} If & v_t = 0 & then & r_t \in [-\mu r_n, \mu r_n] \\ else & & & r_t = -sign(v_t)\mu r_n \end{array}$$

where μ is the local friction coefficient

* an elastic shock law using the new variables

$$(1+e)\bar{\mathbf{v}} = e\mathbf{v}_{free} + \mathbf{v}_{i+1}$$



where **e** is the restitution coefficient (normal and/or tangential)

4. Contact problem resolution

The solution of problem [4] is obtained using a block Non Linear Gauss-Seidel algorithm. During each Gauss-Seidel iteration, local contact forces are determined by solving the problem [4] contact by contact as follow

$$\left\{ \begin{array}{l} \mathbb{W}_{\alpha\alpha} h \mathbf{r}_{\alpha}^{k+1} - \mathbf{v}_{\alpha}^{k+1} = -\mathbf{v}_{free,\alpha} - \sum_{\beta<\alpha} \mathbb{W}_{\alpha\beta} h \mathbf{r}_{\beta}^{k+1} - \sum_{\beta>\alpha} \mathbb{W}_{\alpha\beta} h \mathbf{r}_{\beta}^{k} \\ ContactLaw(\mathbf{r}_{\alpha}^{k+1}, \mathbf{v}_{\alpha}^{k+1}) = true \end{array} \right.$$

The convergence test of the algorithm is performed each N iterations until reached the maximal number of iterations.

The NLGS algorithm is robust but have a slow convergence. Nevertheless, It allow do deal with various contact law as mentioned further.

5. About numerical parameters ...

a - No rule exists to choose the time step of simulation. Nevertheless, the physics of the studied system could be used (microscopic time).

b - The parameter **N** must not be too small to minimize the number of convergence test and must not be too large to minimize the number of additional iterations.

c - During the contact detection (no mentionned here), an alert distance must be defined to avoid numerical overlaping between particles which parasite the quality of the solution.

d - The contact problem have a multiplicity of solution (hyperstatic system). Two ways of reading the contact loop lead to two different local solutions but with the same macroscopic properties.

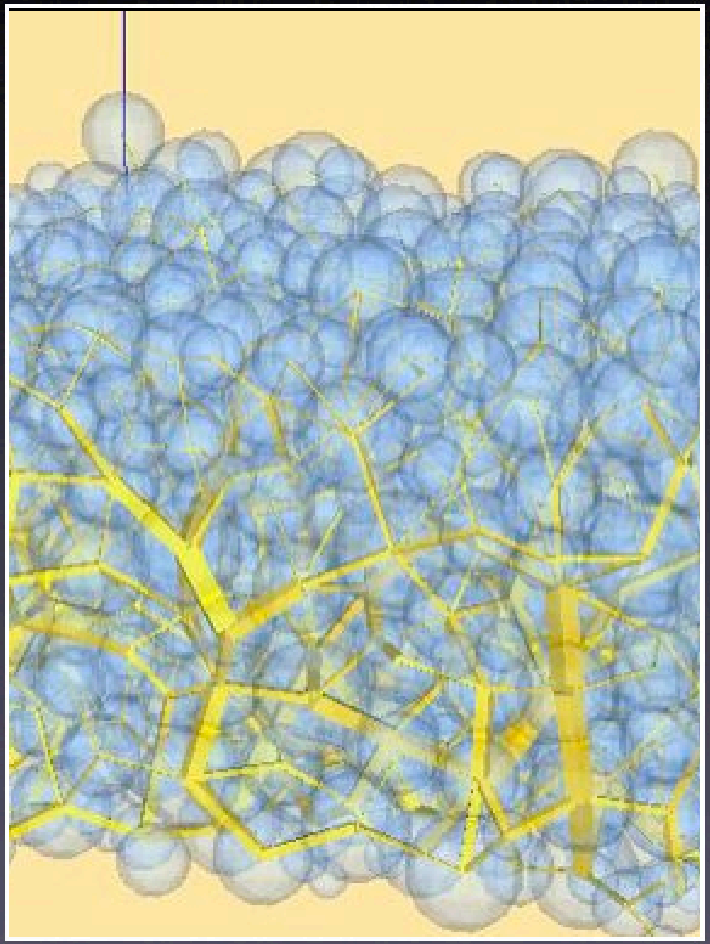
Algorithm development
NSCD optimization

1. Introduction

2. Algorithm

3. Projection definition

4. Numerical results



Contact network in a 3D packing

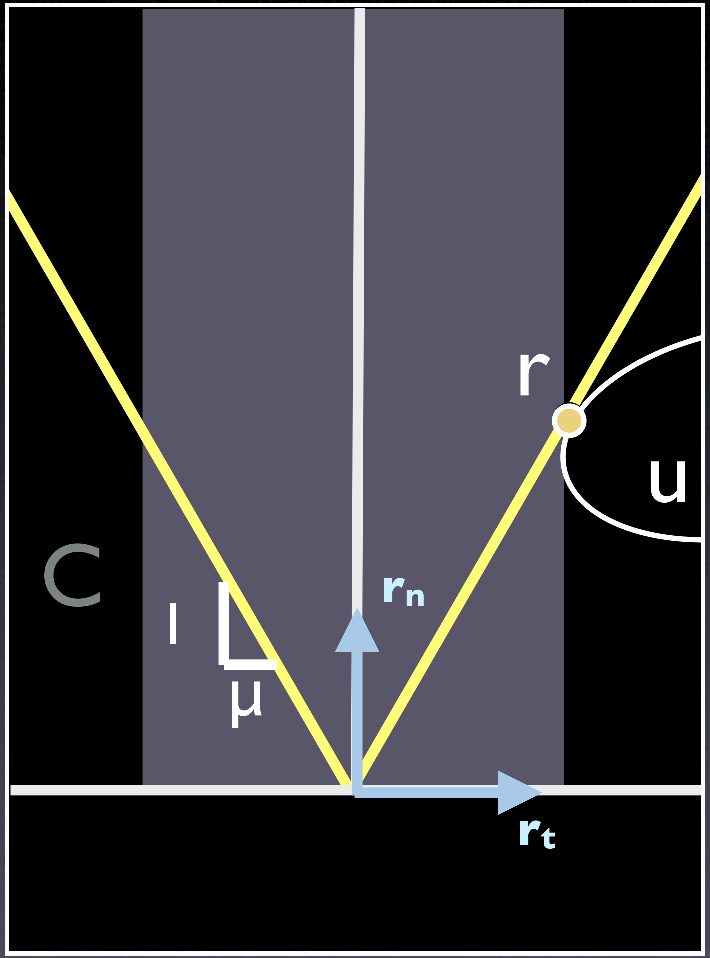
Conjugate Projected Gradient

1. Problem setting

As the NLGS algorithm have a slow convergence a Conjugate Gradient type algorithm have been developed. Their convergences are known to be faster than Gauss-Seidel algorithm (in linear case) and intrinsically parallel.

To adapt gradient type algorithm to friction contact problems, the problem [4] is written as quasi-optimization problem:

$$\mathbf{r} \in \underset{\tilde{\mathbf{r}} \in \mathcal{C}(\mu r_n)}{argmin} \quad \frac{1}{2}\tilde{\mathbf{r}}.\mathbb{W}\tilde{\mathbf{r}} - \mathbf{b}.\tilde{\mathbf{r}}$$



where $C(\mu r_n)$ is the coulomb cone associated to the normal component of the contact forces.

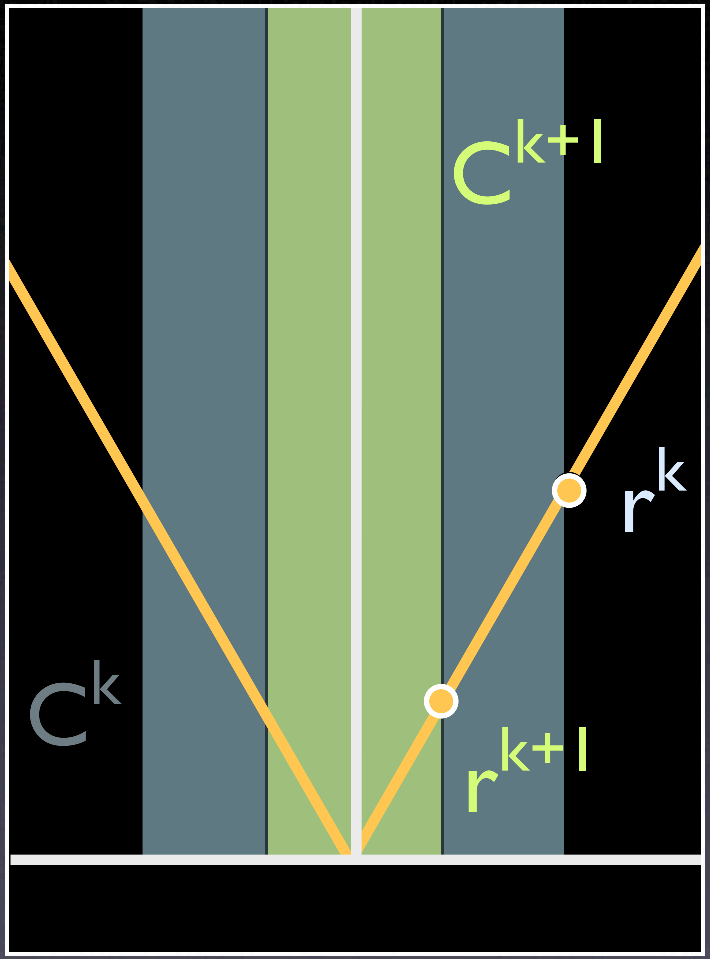
Conjugate Projected Gradient

2. algorithm

To proceed, the algorithm will be the diagonalisation of a fixed point algorithm

$$\mathbf{s}^0 = (\mathbf{s}^0 \geq 0 | \alpha \in \{1, ..., n_c\})$$
$$\mathbf{r}^0 = 0 \ (or\ a\ given\ value)$$
$$l = l + 1$$
$$\left[\begin{array}{lll} \mathbf{s}^l_\alpha & = \mu \mathbf{r}^{l-1}_{\alpha,n} & \text{(a)} \\ \mathbf{r}^{l,0} & = \mathbf{r}^{l-1,conv} & \text{(b)} \\ \mathbf{r}^{l,conv} & = \underset{\mathbf{r} \in \mathcal{C}^l}{argmin} \quad \frac{1}{2}\tilde{\mathbf{r}}.\mathbb{W}\tilde{\mathbf{r}} - \mathbf{b}.\tilde{\mathbf{r}} & \text{(c)} \end{array}\right.$$

(d)



with

(a) Treshold update
(b) Iterate initialization
(c) Tresca problem
(d) iterate projection

3. projection definition (1/2)

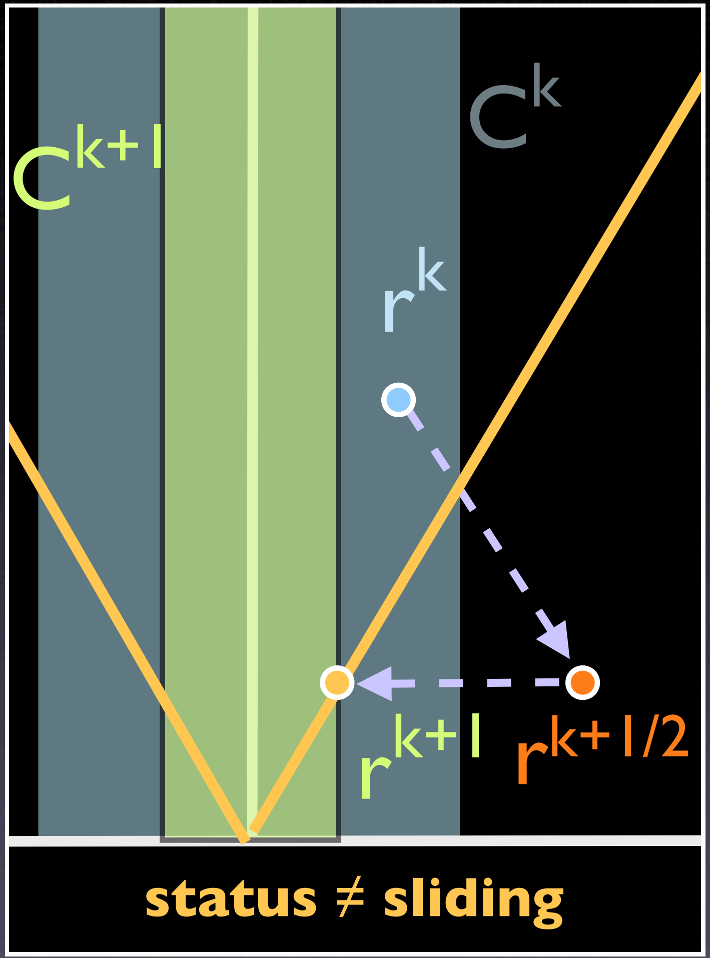
The previous fixed point algorithm is solved by reducing the Tresca problem to a single iteration.

The different projections are operated on the prediction of the iterate as well as on the two gradient:

$$\mathbf{r}^{k+1} = \boxed{Correction}\{\mathbf{r}^k + \alpha^k \mathbf{p}^k\}$$

where

$$\mathbf{p}^k = \boxed{proj}(\mathbf{u}^k; T_{\mathcal{C}^k}(\mathbf{r}^k)) + \beta_k \boxed{proj}(\mathbf{p}^{k-1}; T_{\mathcal{C}^k}(\mathbf{r}^k))$$



Conjugate Projected Gradient

3. projection definition (2/2)

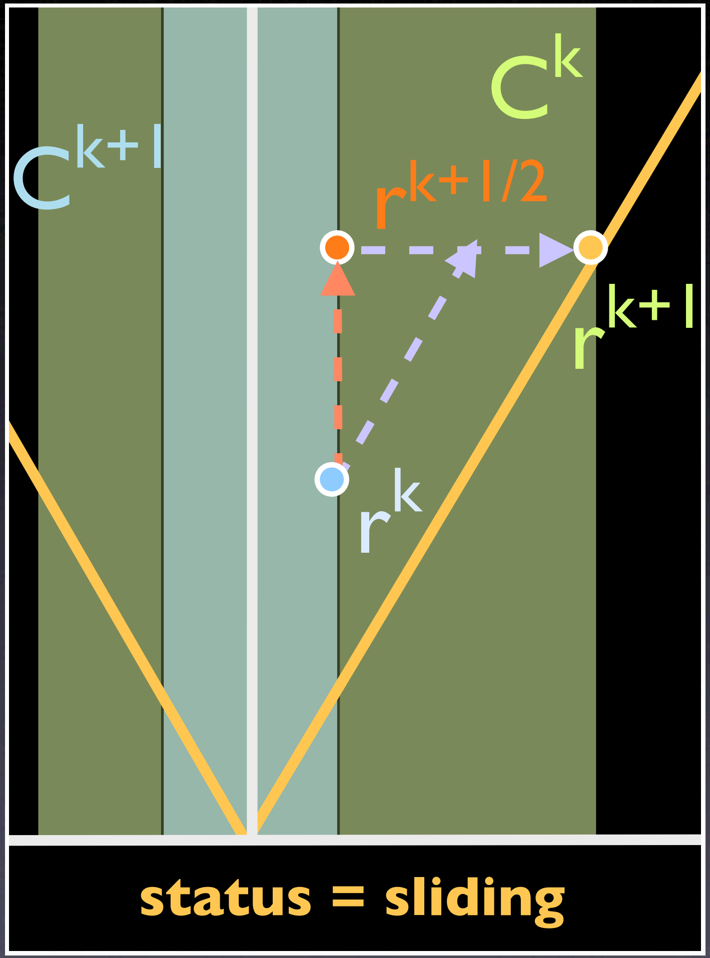
The previous fixed point algorithm is solved by reducing the Tresca problem to a single iteration.

The different projections are operated on the prediction of the iterate as well as on the two gradient:

$$\mathbf{r}^{k+1} = \boxed{Correction}\{\mathbf{r}^k + \alpha^k \mathbf{p}^k\}$$

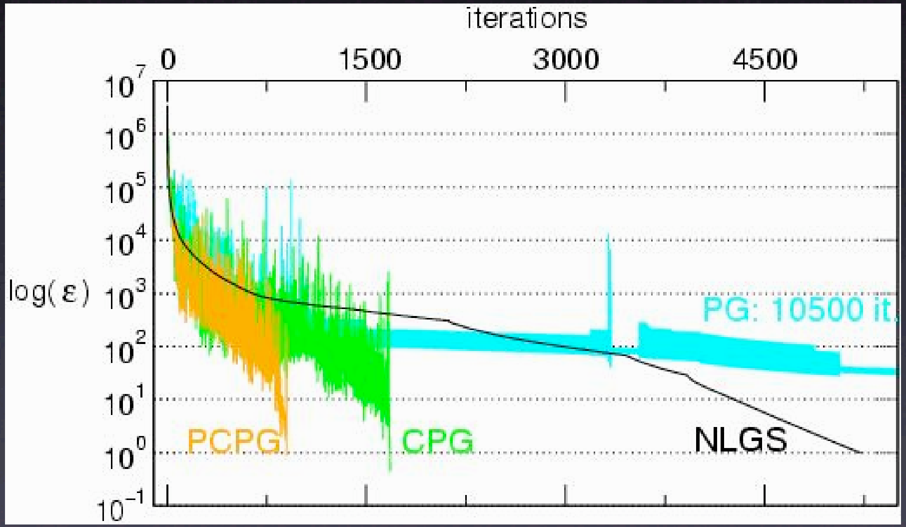
where

$$\mathbf{p}^k = \boxed{proj}(\mathbf{u}^k; T_{\mathcal{C}^k}(\mathbf{r}^k)) + \beta_k \boxed{proj}(\mathbf{p}^{k-1}; T_{\mathcal{C}^k}(\mathbf{r}^k))$$



4. Numerical results (1/5)

On a single time step



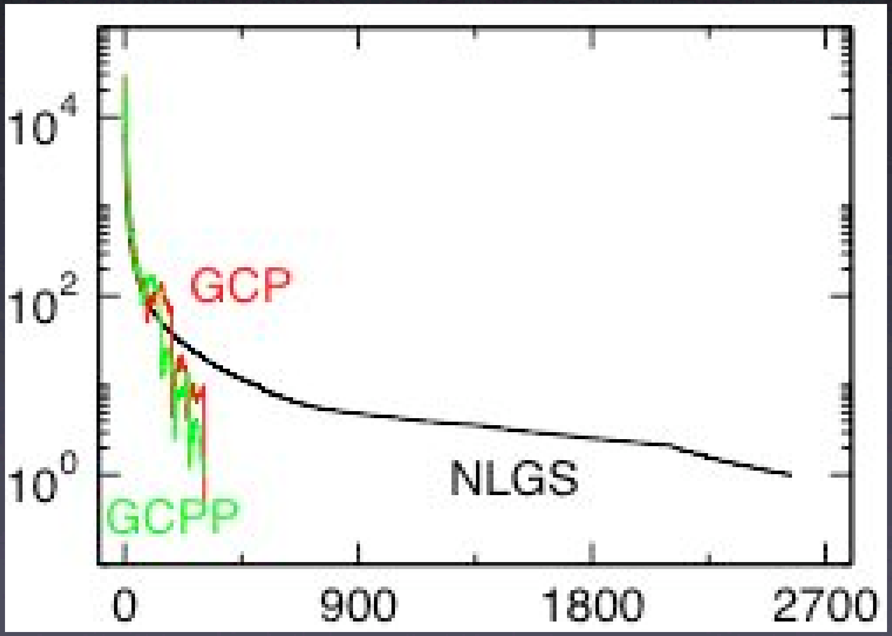
Evolution of the error criterium during the iterative process for the NLGS, PG, CPG and PCPG algorihtms for the resolution of a contact problem (μ = 0.1),

Fast convergence in regard of the NLGS and the gradient without conjugaison. Moreover using a simple diagonal preconditionner accelerate the convergence of the initial conjugate projected gradient algorithm.

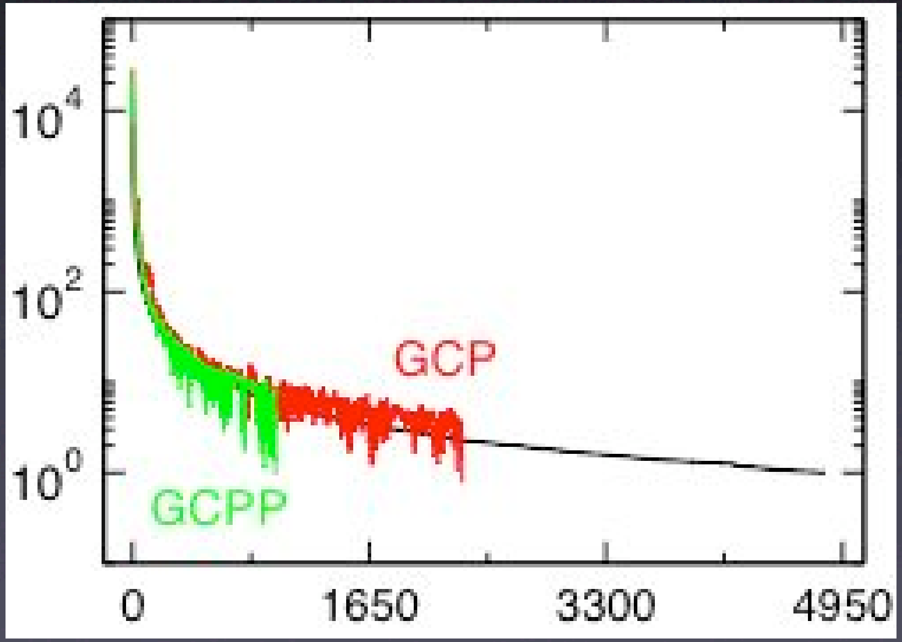
4. Numerical results (2/5)

On a single time step

Influence of the friction coefficient on the algorithm convergence.



μ = 0.0

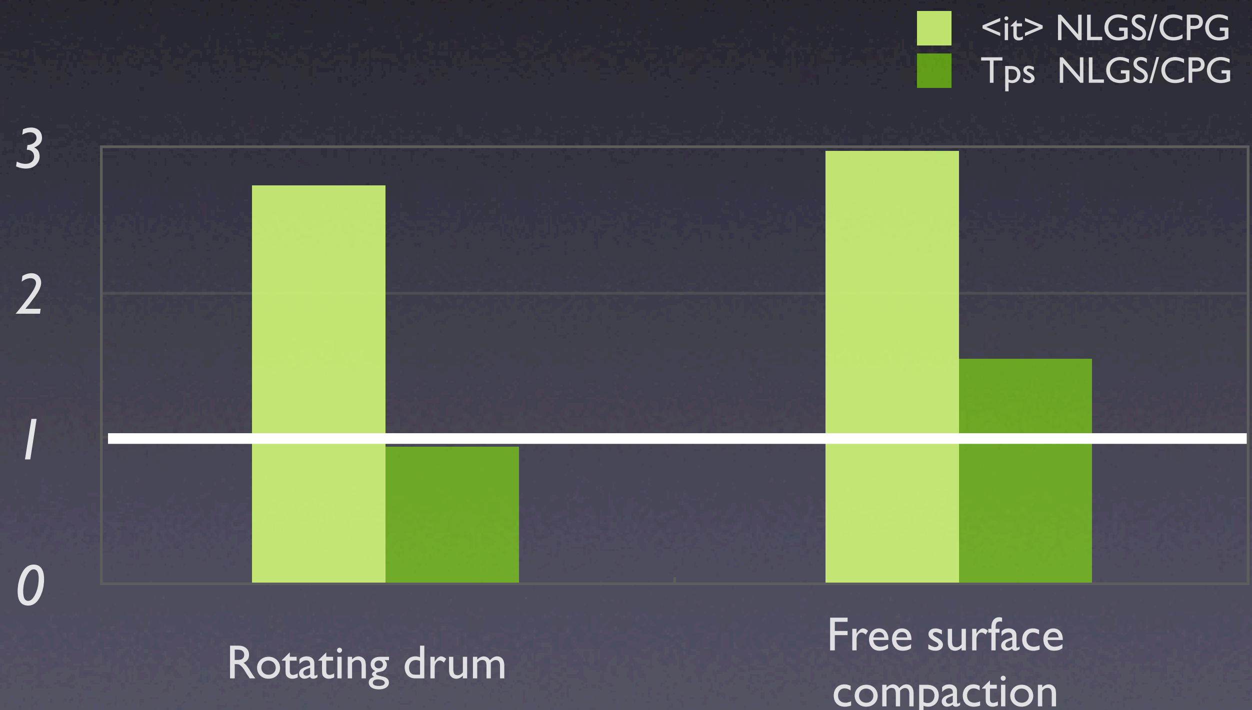


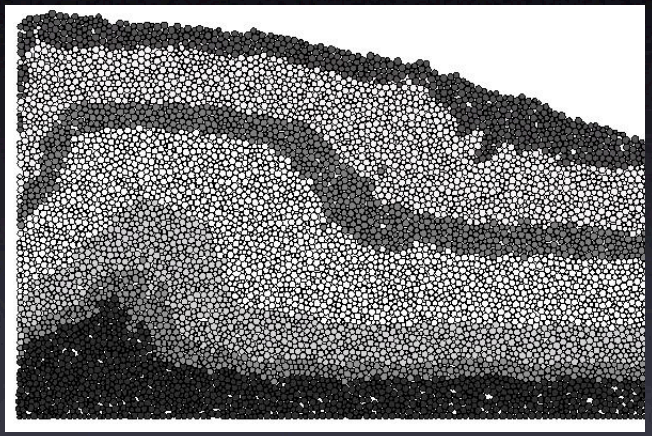
μ = 0.4

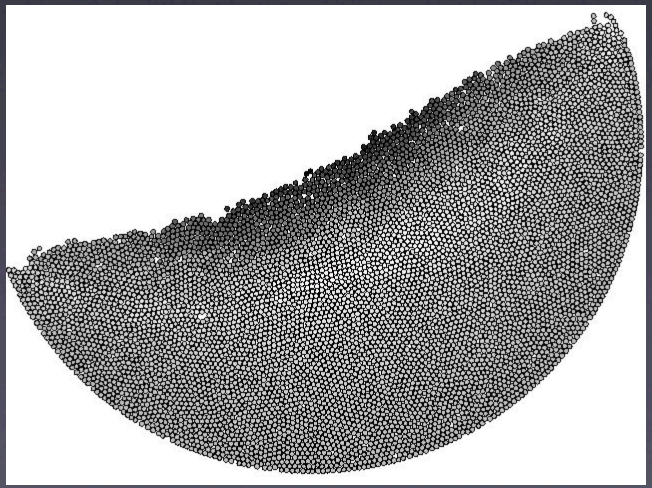
4. Numerical results (3/5)

During the whole process

Behaviour of the CPG algorithm for quasi-static and dynamic process





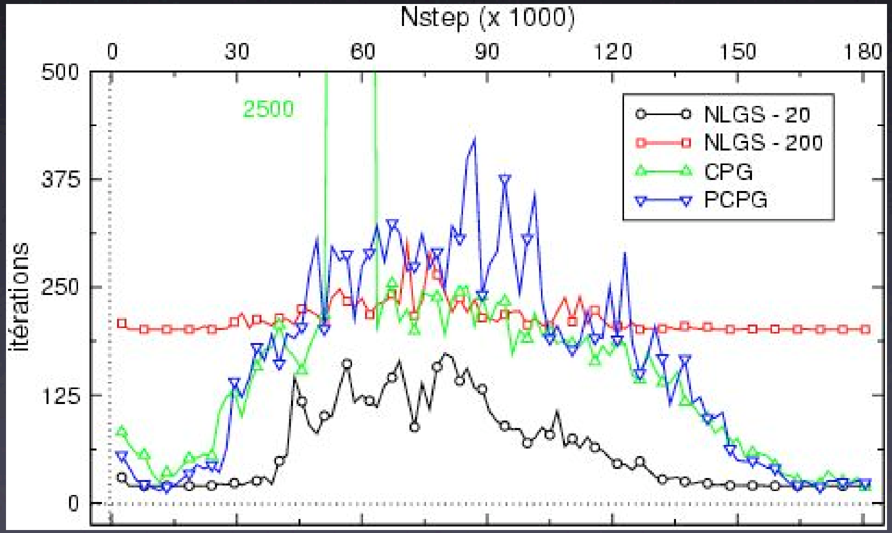


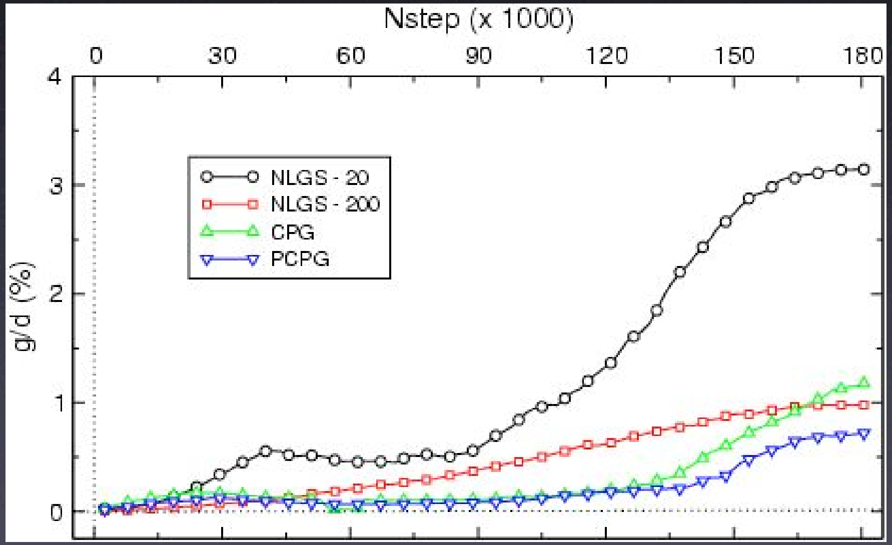
Conjugate Projected Gradient

4. Numerical results (4/5)

During the whole process

Evolution of iteration number and comparison of the quality of the solution.





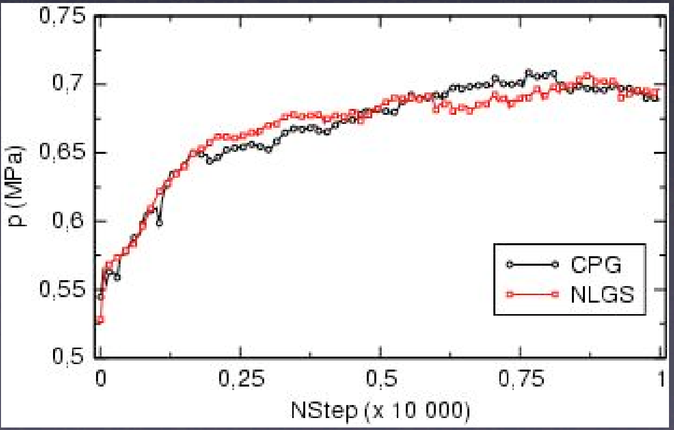
The convergence test of NLGS algorithm is performed each N

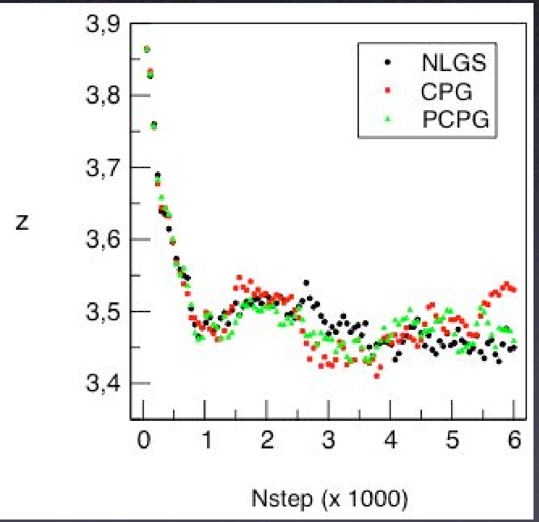
4. Numerical results (5/5)

During the whole process

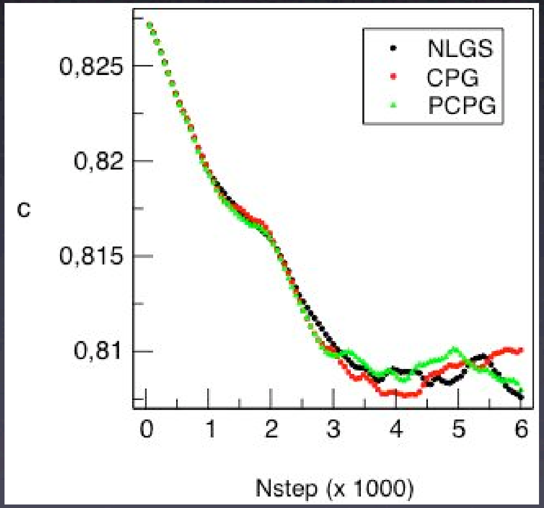
Comparison of macroscopic properties during a bi-axial test

Evolution
of the pressure in the sample



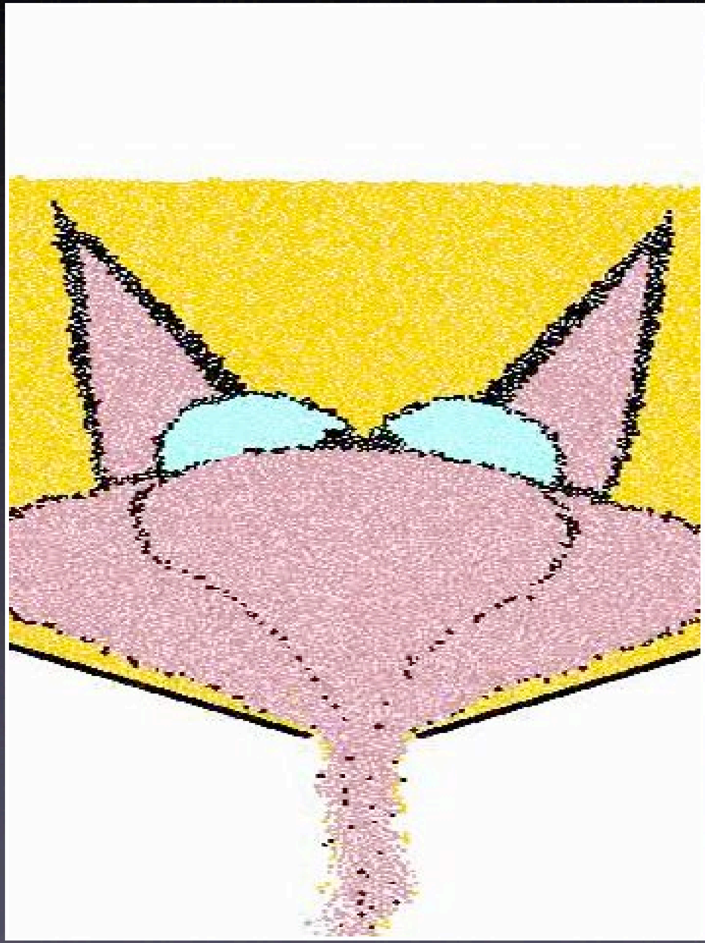


evolution of the coordinence



evolution of compacity

Some simulation results

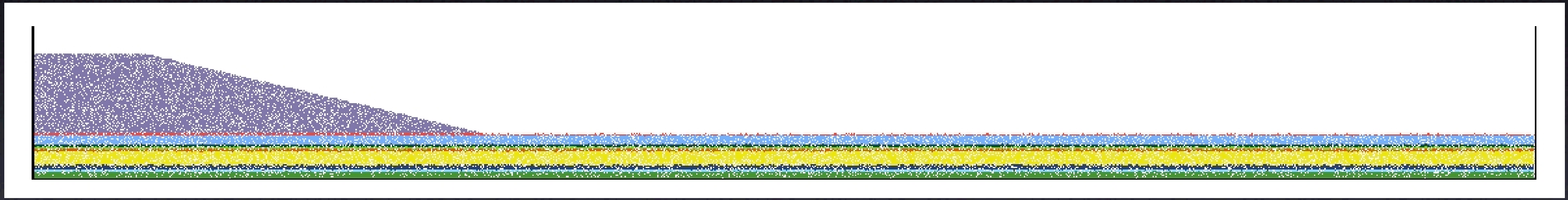


Silo draining simulation snapshot

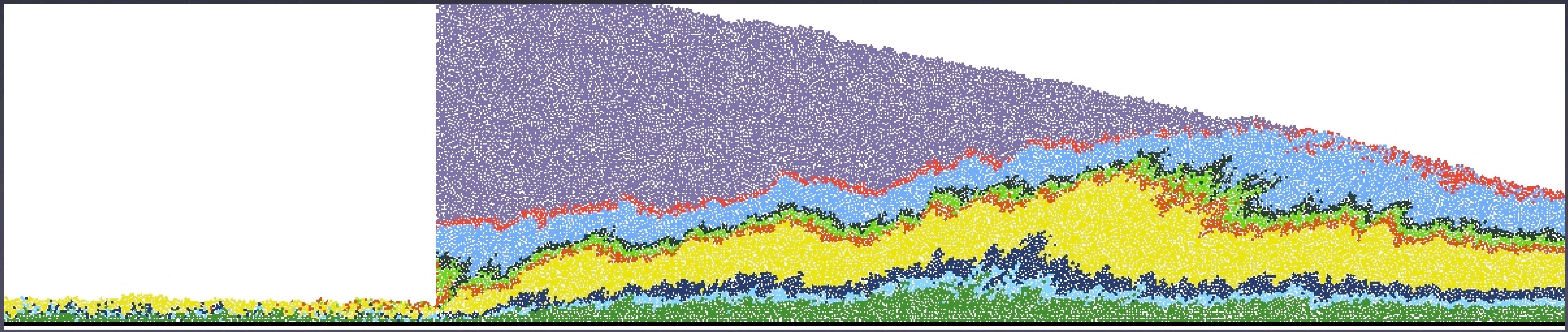
Geophysics *Fault and Fold propagation*

Examples of simulations

initial configuration

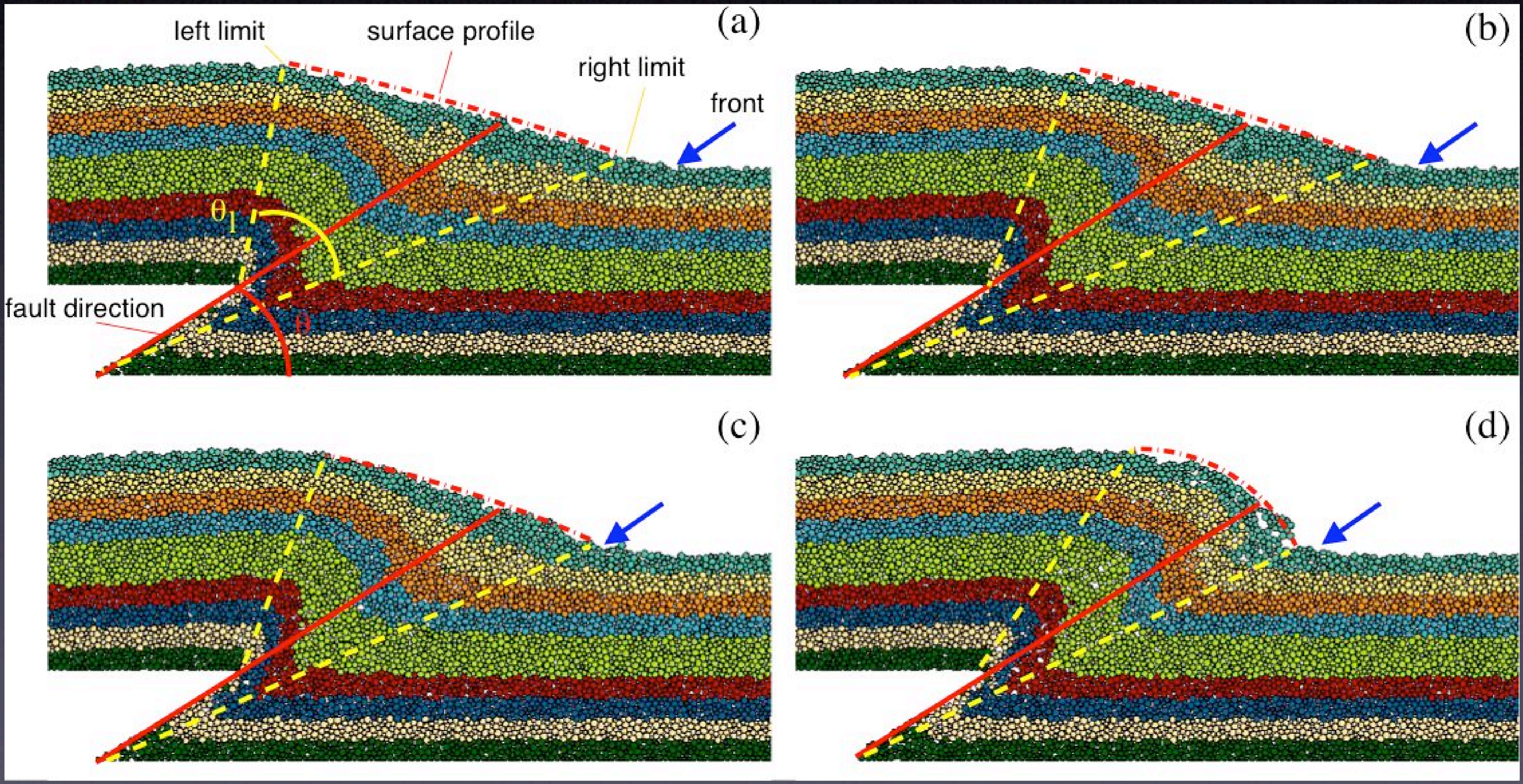


snapshot during the compaction process



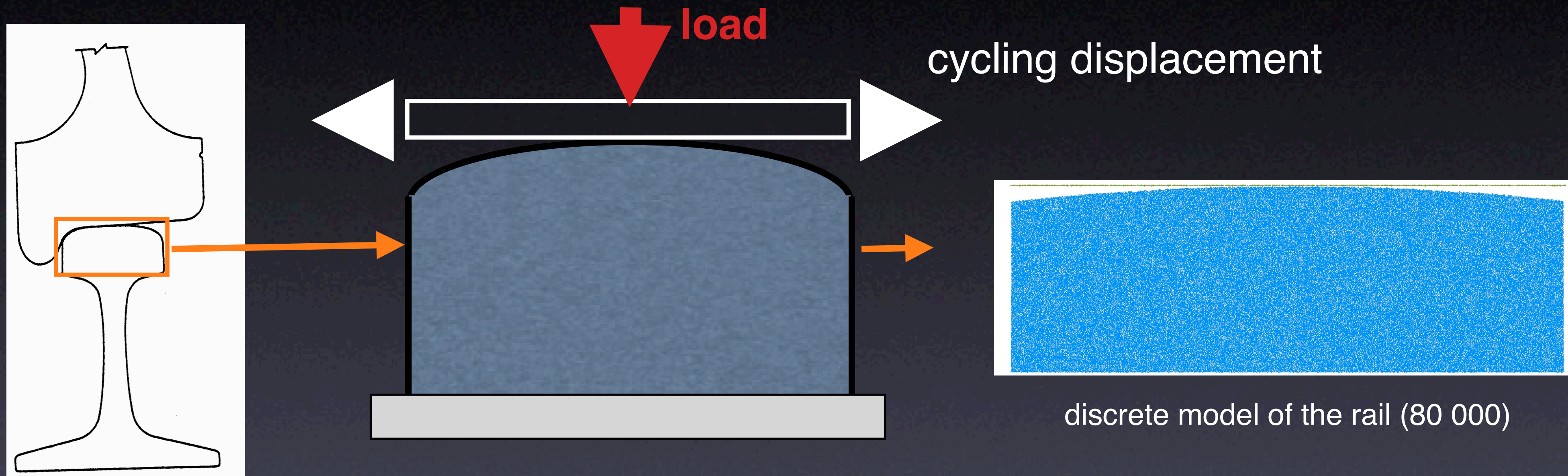
Geophysics *Fault and Fold propagation*

Propagation fault: influence of internal cohesion



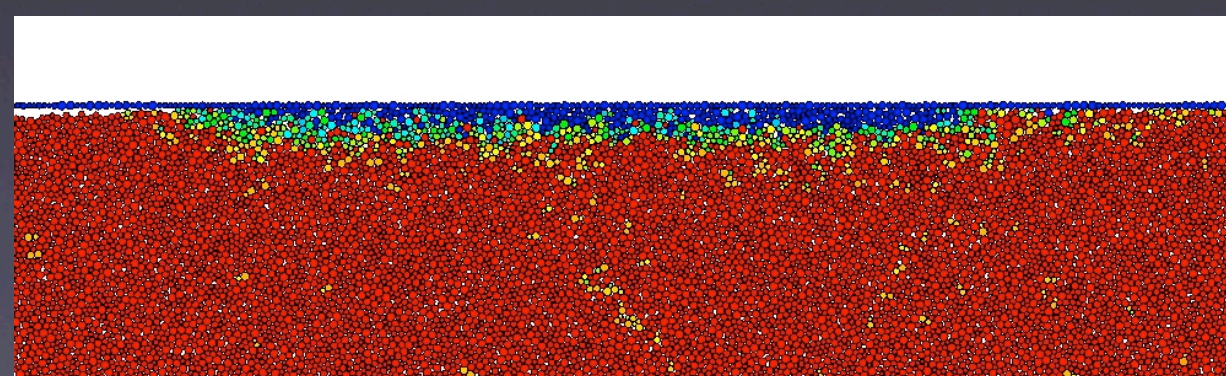
Tribology ***third-body rheology***

Third-body flow during wheel-rail interaction under fretting sollicitations



discrete model of the rail (80 000)

Wear visualisation:
- all interactions of red particles are undamaged
- all interactions of blue particles are damaged

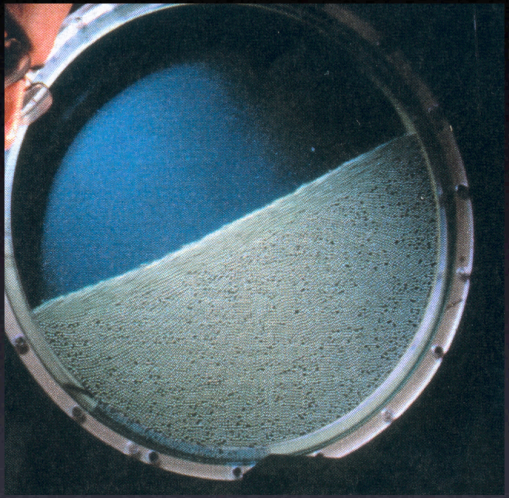


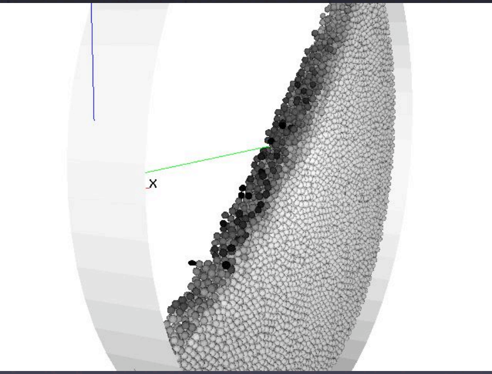
Granular flow rotating drum

Investigation of the rheology of 2D and 3D surface flow:

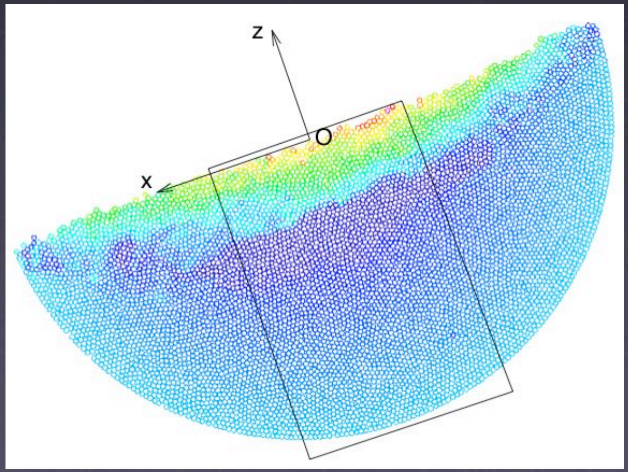
- description of surface flow rheology (2D)

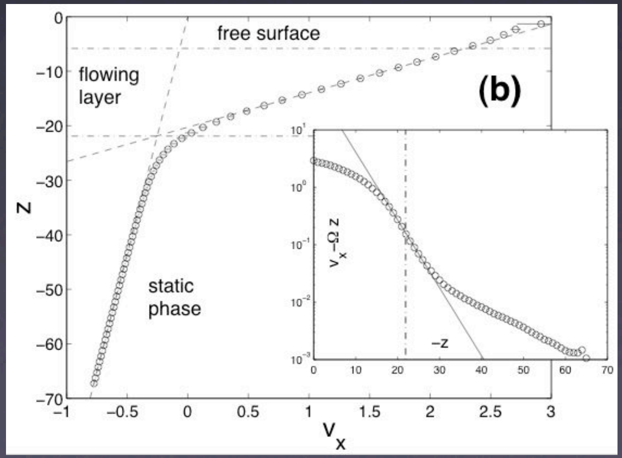
- underlining influence of the lateral wall (3D)





threedimensional rotating drum used for the investigation of lateral friction





Left: Typical 2D snapshot to study free surface flow (visualisation of the velocity field). Right: velocity profile at the center of the drum.

Conclusions

What about the future of divided media !?

As divided media are still around us, and their behaviour is not yet understood in some circunstances, DEM will not become an has been approach.

If the pure mechanical approach benefit of numerous approach (MD, DEM, CD), combined approach need to develop new algorithm to understand the multi-physics feature of some discontinuous assemblies (thermal, electrical,...)

Finally as in some circunstances, the divided feature of media is evolutive, new strategy must be developped to face this evolutive process (wear, fissuration,...)