

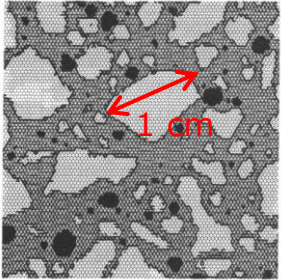
# About Discrete Element modeling in EPX

S. Potapov (EDF R&D/ERMES)

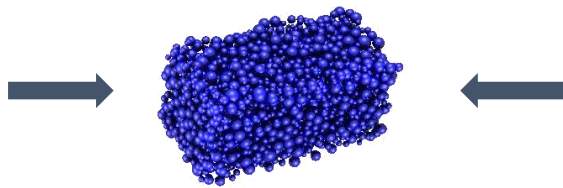
EPX Users meeting, Bruxelles, 06 Juin 2023

# Spherical Discrete Element Method

Material scale

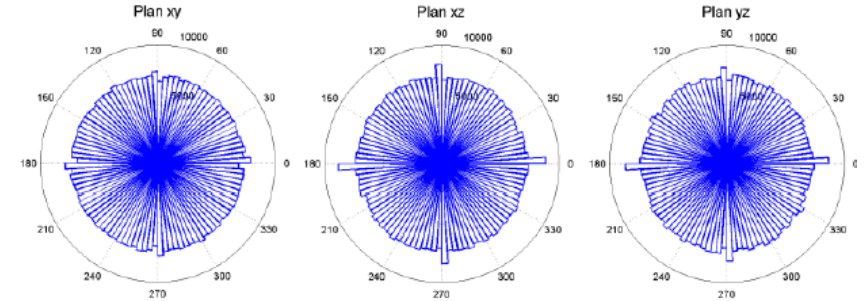


Structure scale

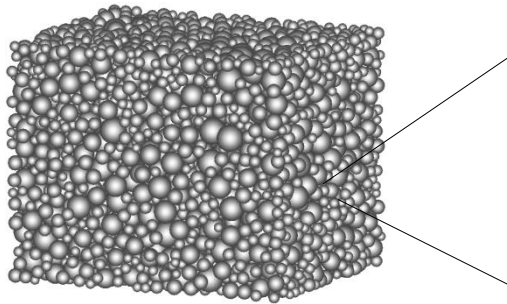


Intermediate modeling scale  
representative of the  
macroscopic behavior

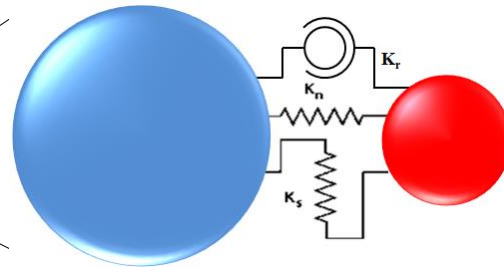
Initial isotropy



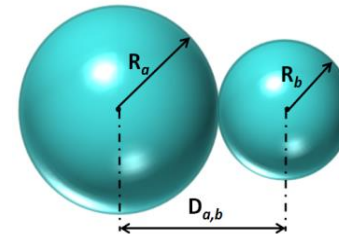
$E, \nu$



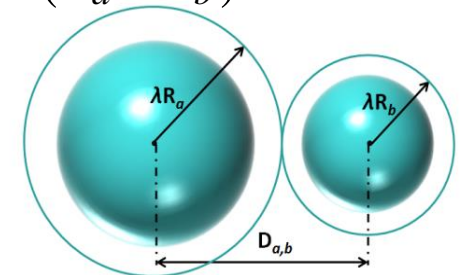
$K_n, K_s, K_R$



Interactions  $\lambda(R_a + R_b) \geq D^{a,b}$



Contact Interaction,  $\lambda = 1$



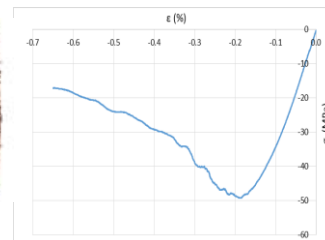
Cohesive Interaction,  $\lambda > 1$

Micro-macro relations

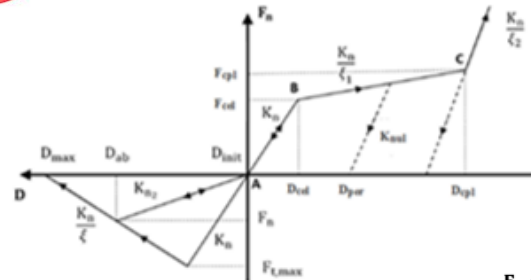
$$\begin{cases} K_N = E \frac{S_{int}}{D_{eq}} \frac{1+\alpha}{\beta(1+\nu)+\gamma(1-\alpha\nu)} \\ K_S = K_N \frac{1-\alpha\nu}{1+\nu} \end{cases}$$

$\alpha, \beta, \text{ et } \gamma$  must be  
identified only once

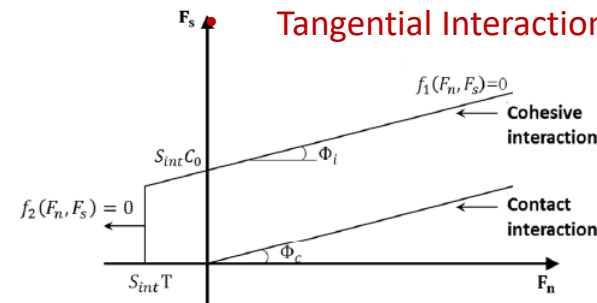
$F(t)$



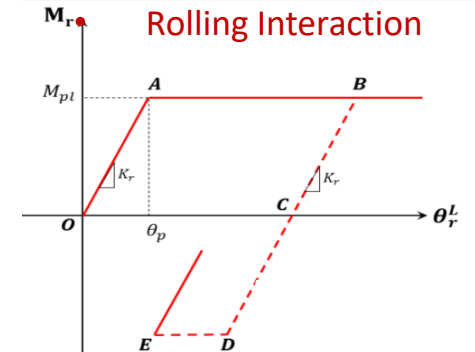
Normal Interaction



Tangential Interaction

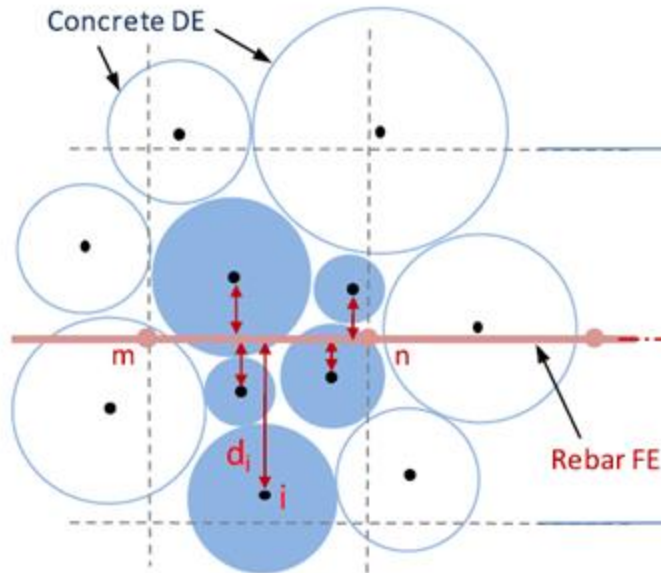
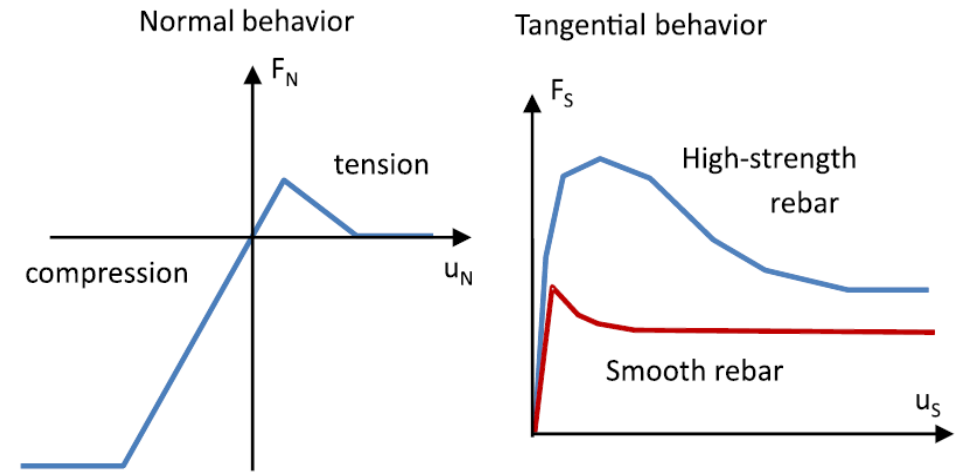
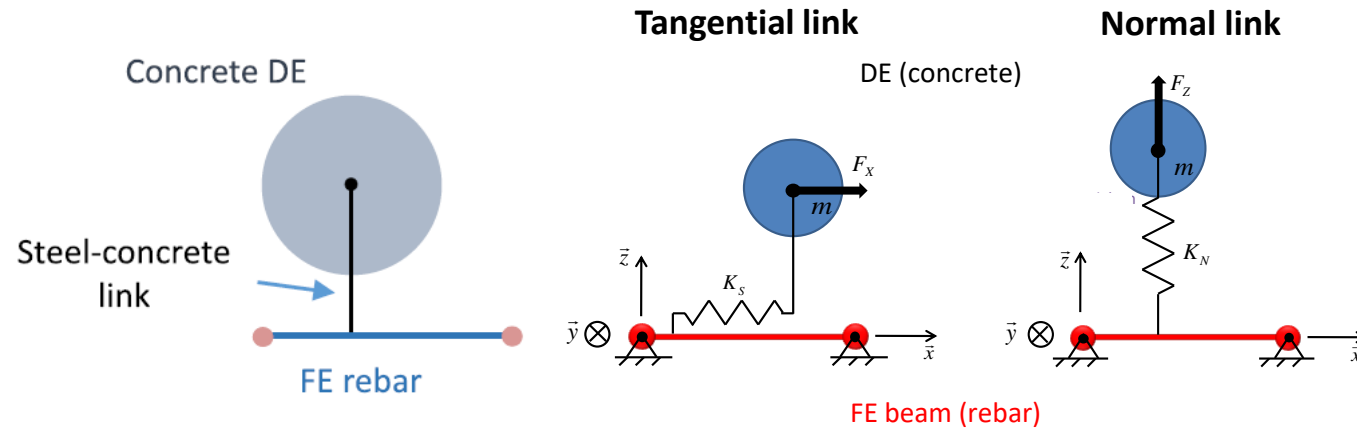


Rolling Interaction

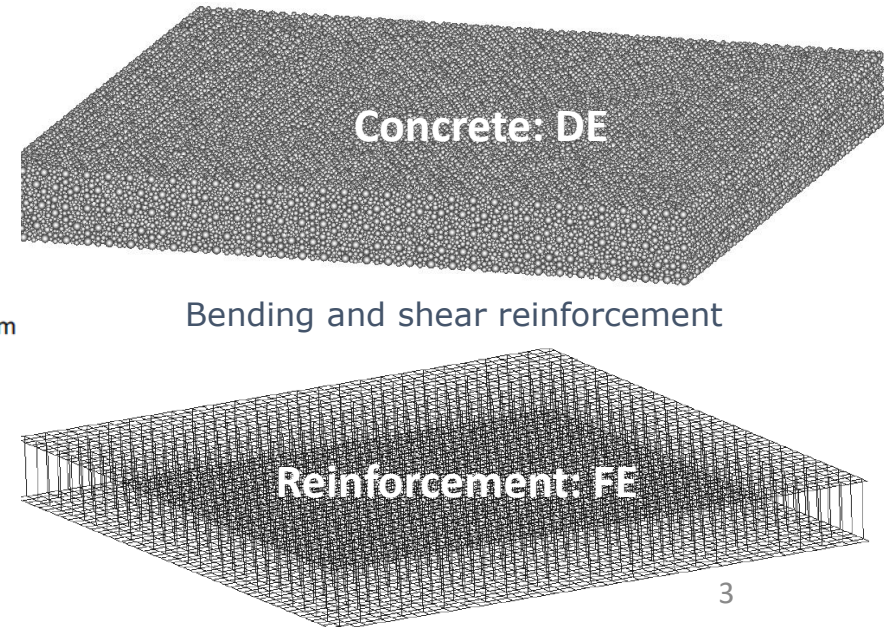
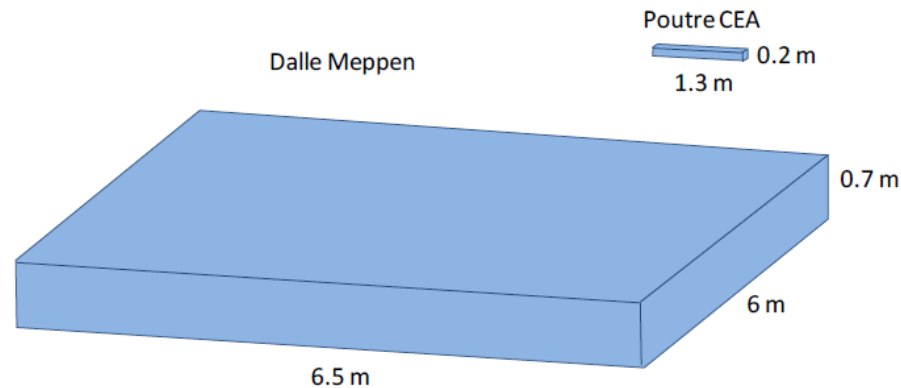


# Steel reinforcement model

- **DE** modeling for **concrete**
- **FE beam** modeling for **rebars**



## Industrial size structure

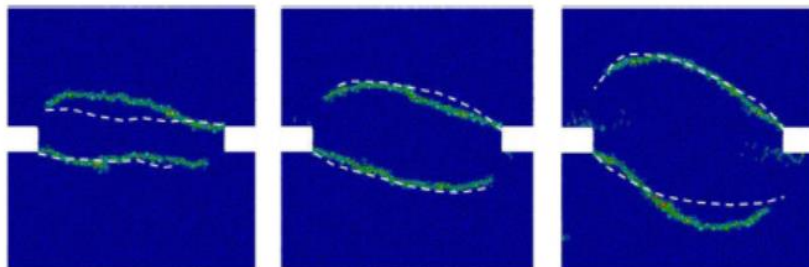




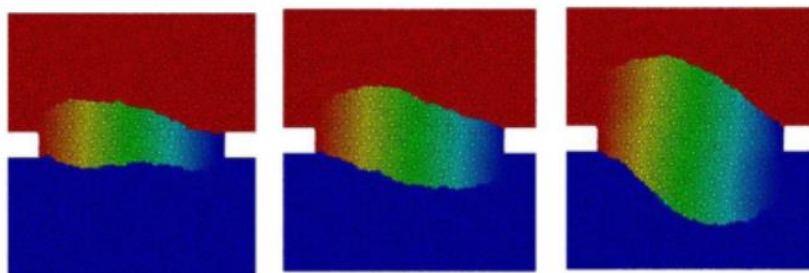
# Simulations of plain and reinforced concrete structures

## Tension-shear experiment

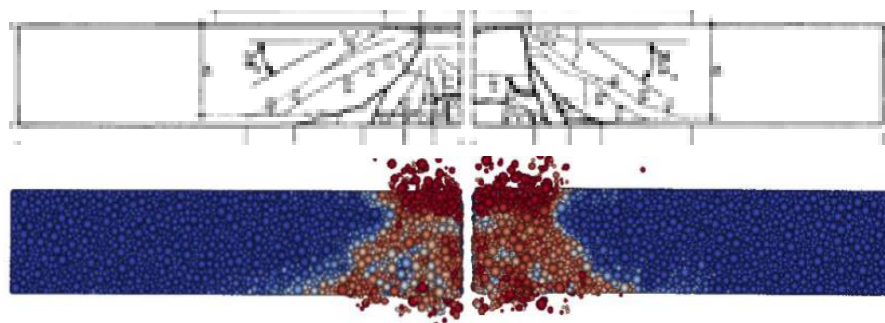
Damage path (broken links)



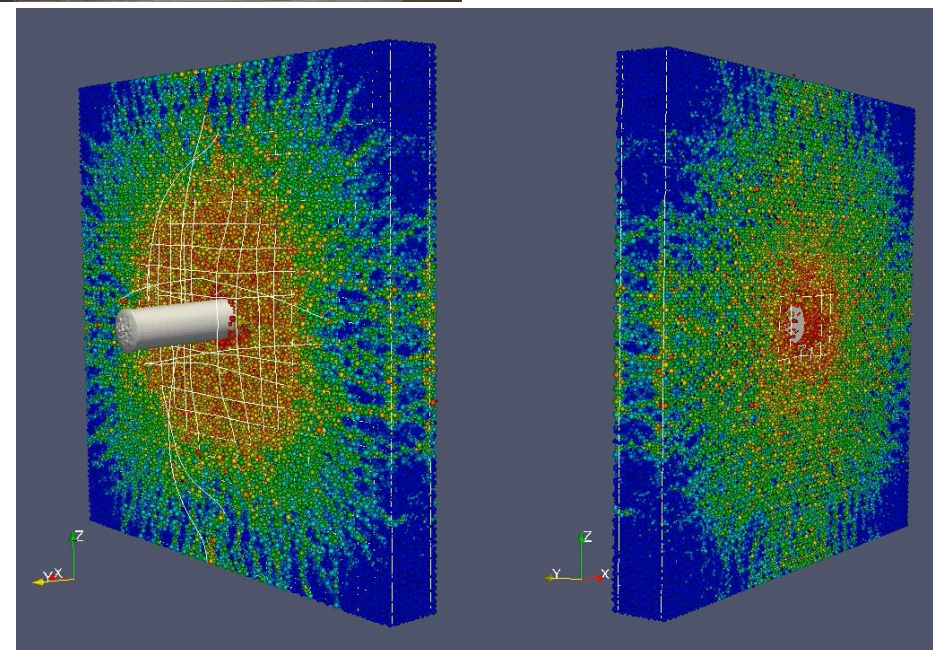
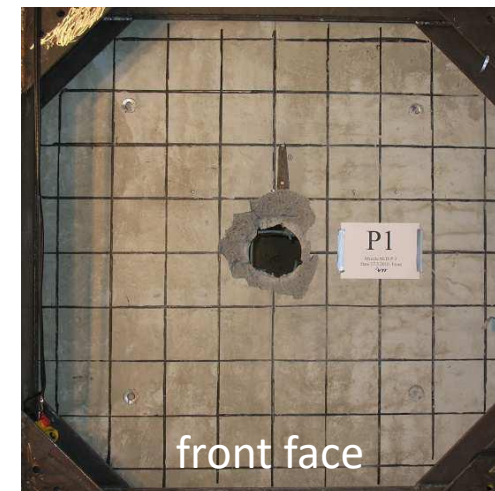
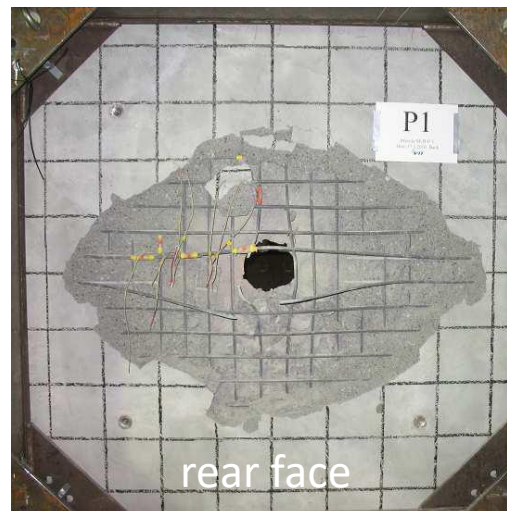
Vertical displacement



## Meppen-IV (impact with damage)

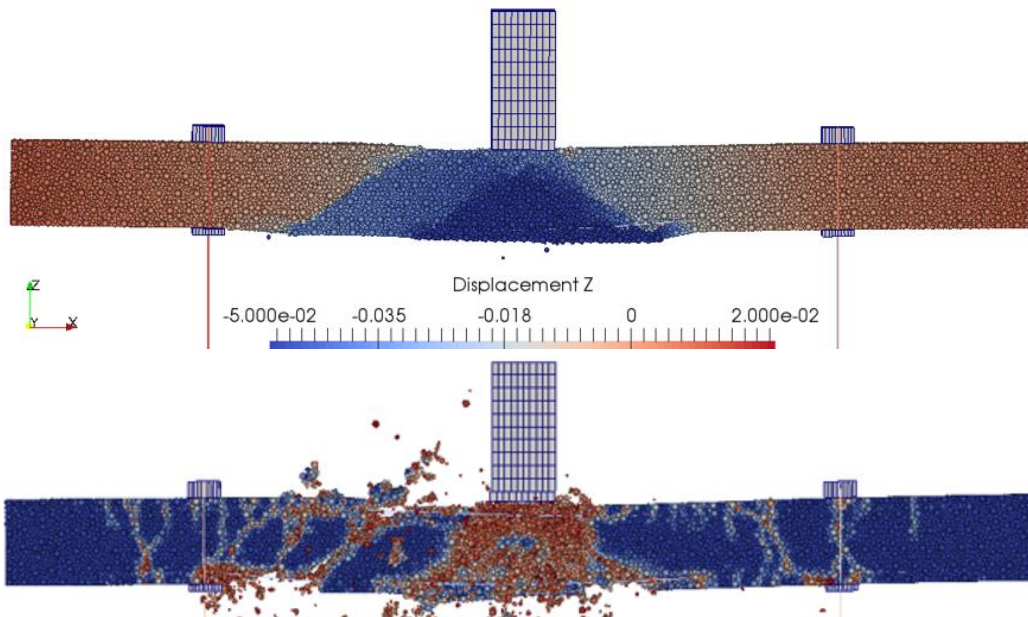
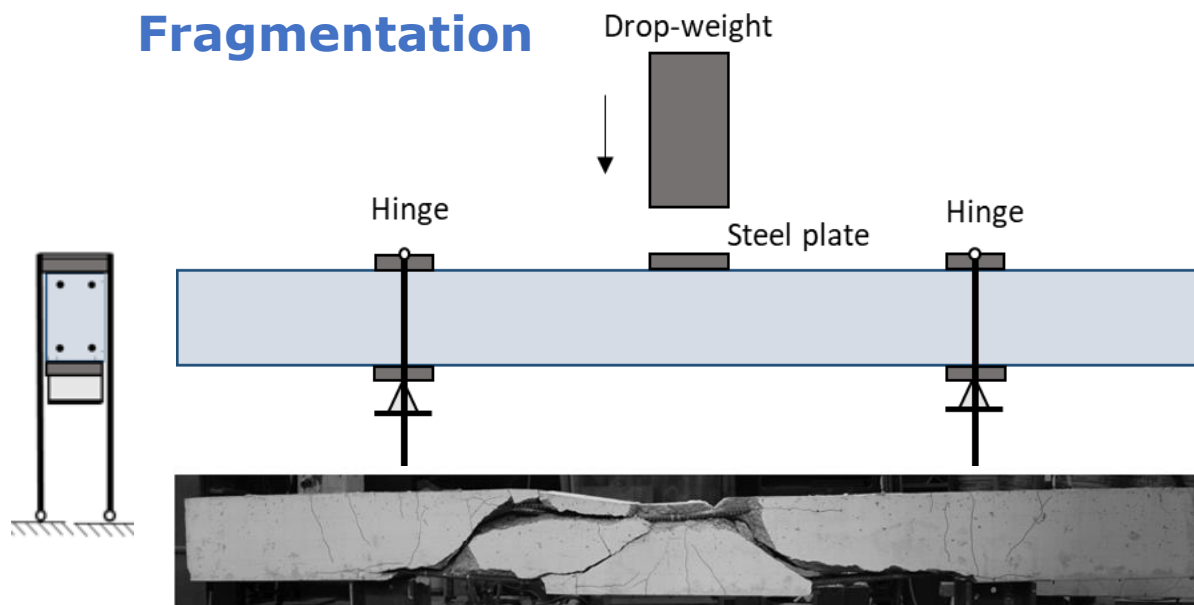


## VTT P1 perforation test

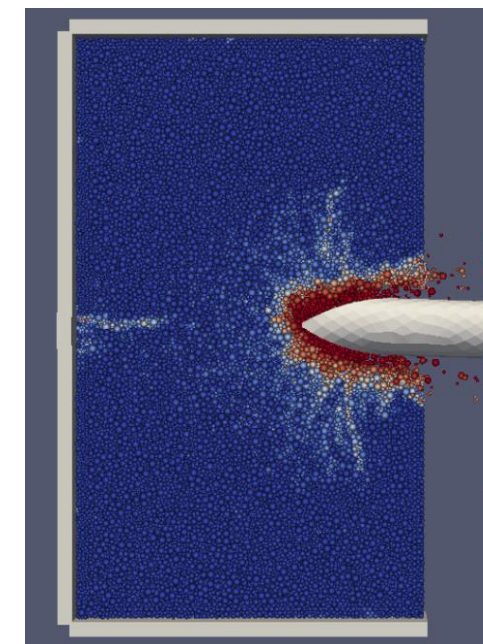
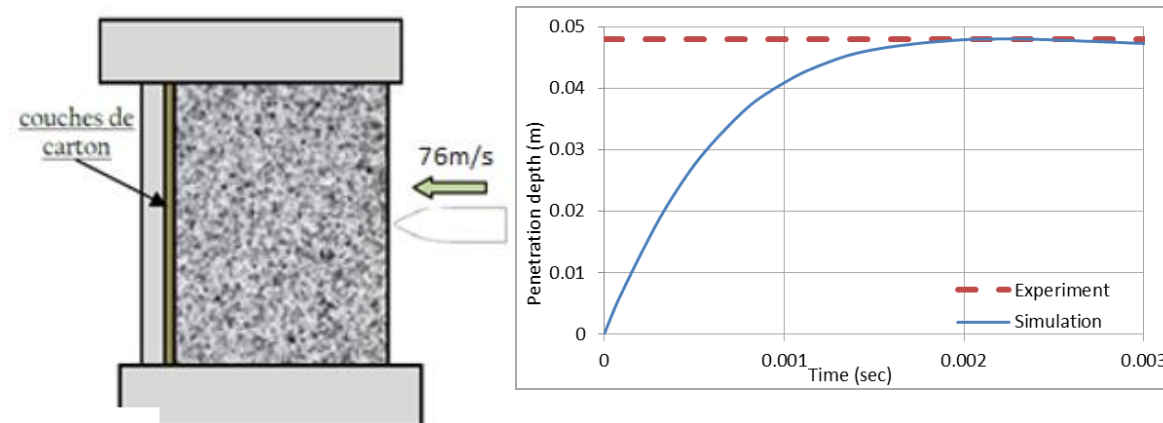


# Simulations of plain and reinforced concrete structures

## Fragmentation



## Penetration of rigid projectile





# Loss of Coolant Accident (LOCA)

## 1) Fuel state evolution in normal operating conditions

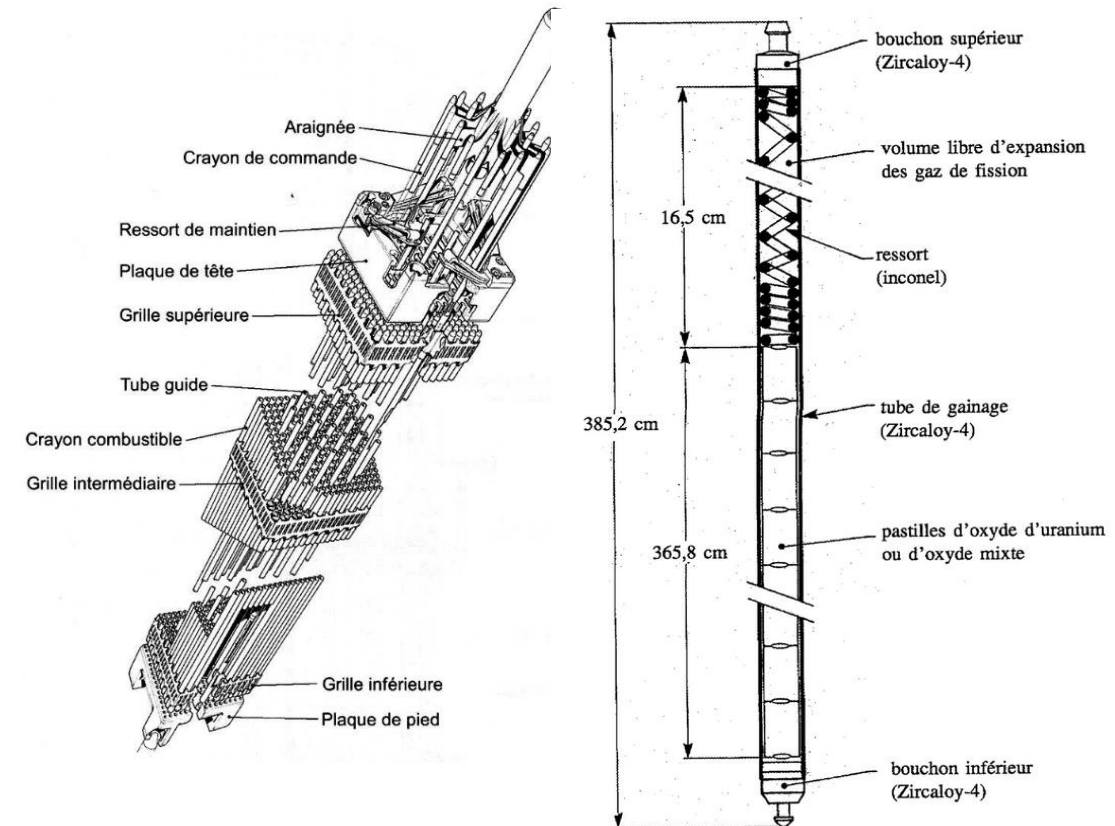
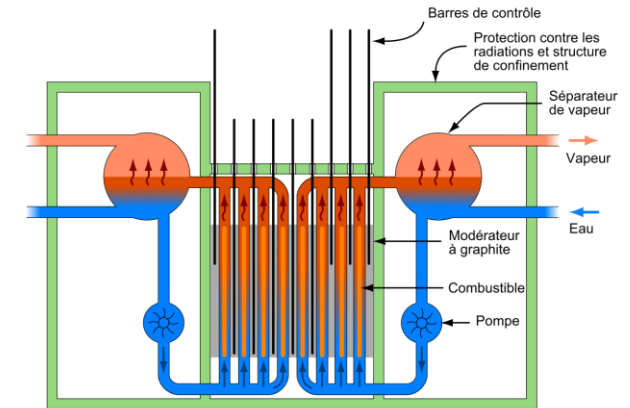
→ **New fuel**: 20 bars helium pre-pressurised rod with 155 bars pressure in the primary fluid outside the cladding tube

→ **First rise in power**:

- Fuel pellets dilation
  - Diabolo-shape deformation
  - First fracturing (*cracking*) of pellets and radial fragments relocation
- => fuel-cladding gap decreasing

→ **1<sup>st</sup> and 2<sup>nd</sup> cycles**: gap closing, folds creation, fuel – cladding interaction

→ **3<sup>rd</sup> and 4<sup>th</sup> cycles**: swelling and creep of the fuel that deforms the cladding



**Cladding**: first confinement barrier between radioactive fuel and the outside environment

# Loss of Coolant Accident (LOCA)

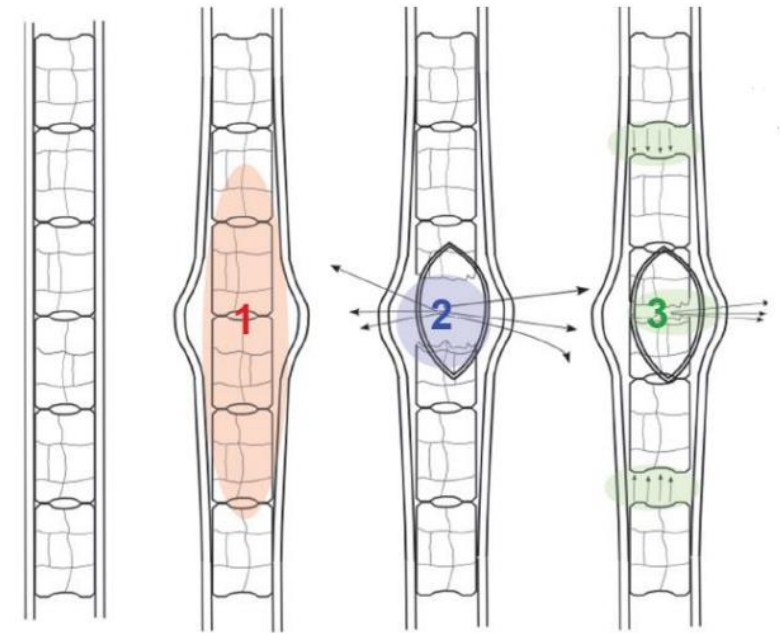
## 2) Fuel rod behavior during LOCA

1. {
  - Outside depressurization and fission gas pressure increases inside the cladding tube => large pressure difference ( $\Delta P = P_{\text{int}} - P_{\text{ext}}$ ) => **Deformation/ swelling of the cladding tube**
  - **Temperature increase in the cladding**

Plastic instability, local **ballooning** => **relocation** of fragments in the ballooned zone

2. **Eventual break-up of the cladding** => loss of fission gas, inside depressurization and additional fragmentation of the primary fragments

3. **Ejection of fragments** outside the cladding



Evolution de l'état du crayon combustible (gaine + combustible) lors du transitoire thermique APRP.

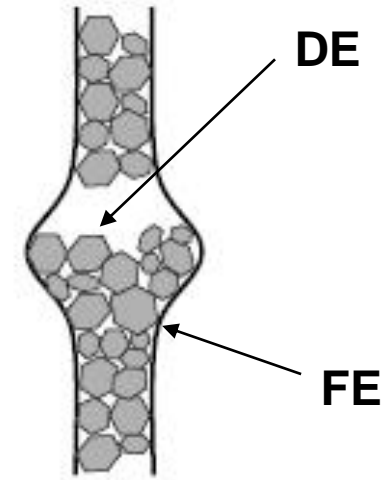
# Need of numerical modeling to complete experimental studies

**Objective:** to build a 3D model accounting for fragments interactions, their over-fragmentation, fragments – cladding and fragments – fluid interactions, etc.

## *Which modeling to choose?*

Discrete element method: widely used to granular media:

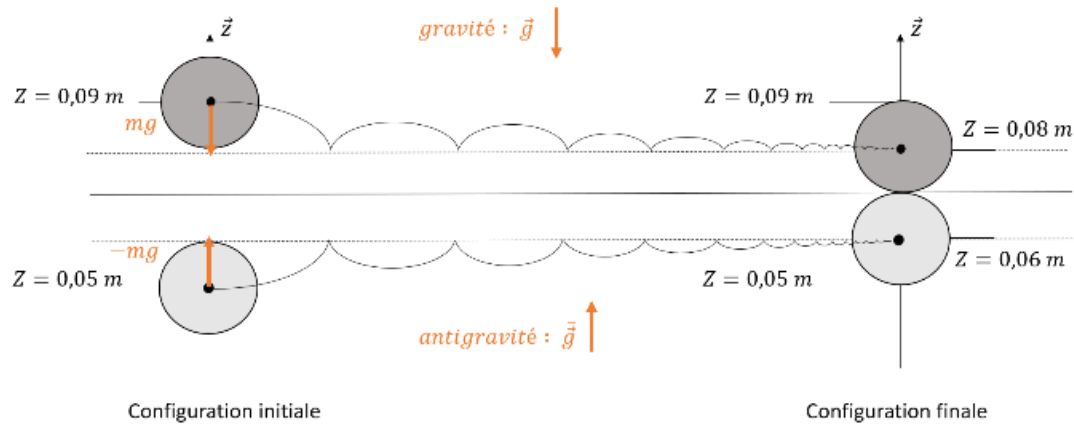
- Accounting for contacts, friction, rolling, different couplings
- Robust, performant and easy to implement



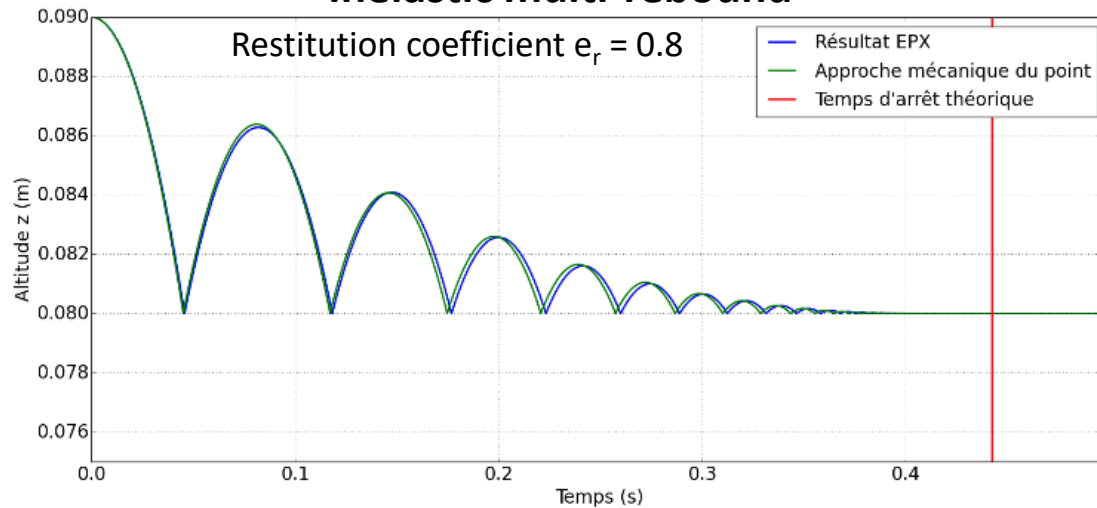


# Normal and tangential interactions modified

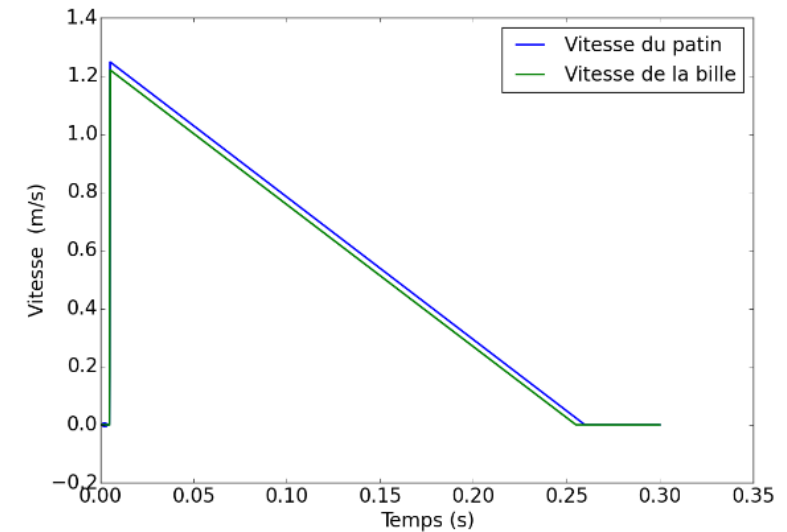
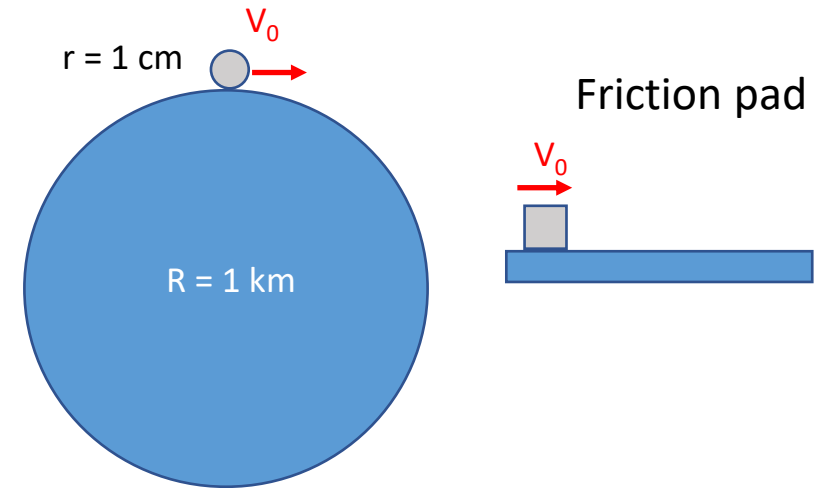
## Inelastic normal collision



## Inelastic multi-rebound



## Tangential interaction with friction

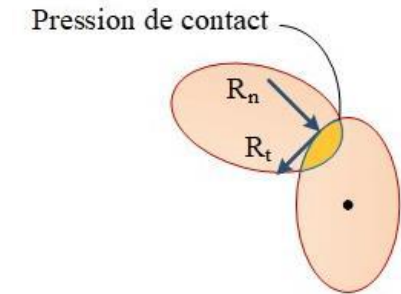


# Rolling resistance

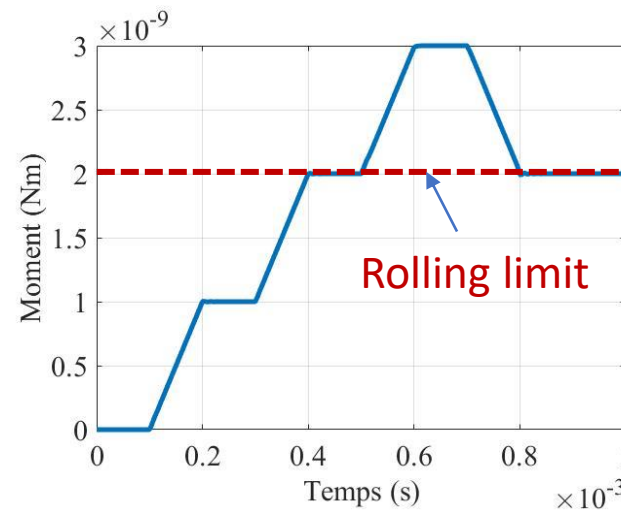
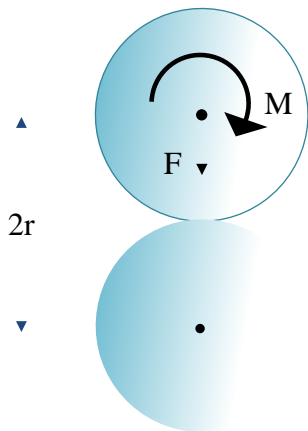
- Maximum rolling torque

$$M_r = \text{sign}(-K_r \theta_r) \mu_r r_{\min} R_n$$

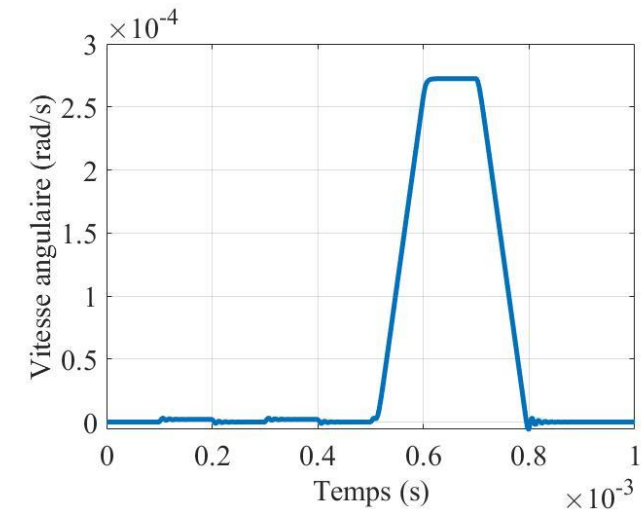
- Modification of rolling coefficient  $\mu_r$  to account for a non spherical shape of grains
- Calibration of rolling resistance for a spherical shape



## Rotational particles interaction



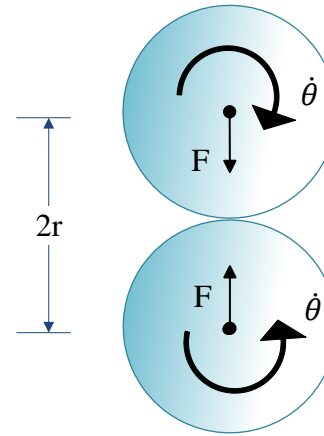
loading



result

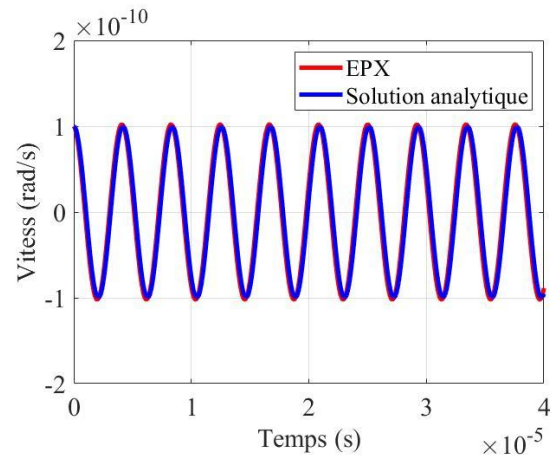
# Rolling damping

$$\eta_r = \frac{C_r}{C_r^{crit}} = \frac{C_r}{2\sqrt{I_r K_r}}$$

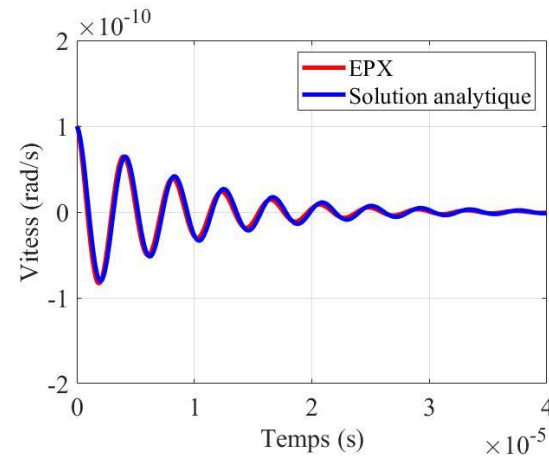


variables	valeur
diamètre	0,002 m
masse volumique	2500 kg/m <sup>3</sup>
module de Young	$20 \times 10^9$ N/m <sup>2</sup>
coefficient de Poisson	0,2
coefficient de restitution	0,87
coefficient de friction	0,5
coefficient de roulement	0.2

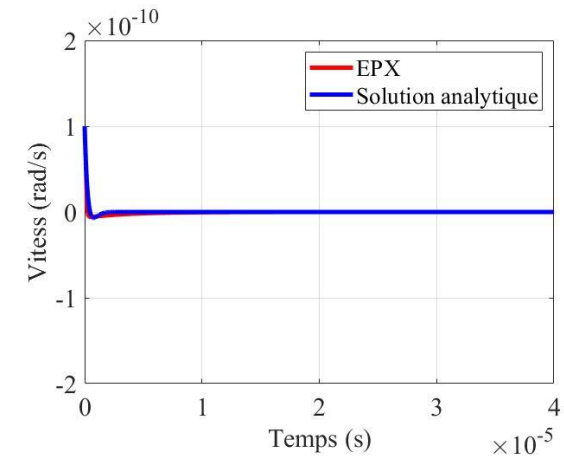
undamped:  $\eta_r = 0$



subcritical damping:  $\eta_r = 0,07$



critical damping:  $\eta_r = 1$

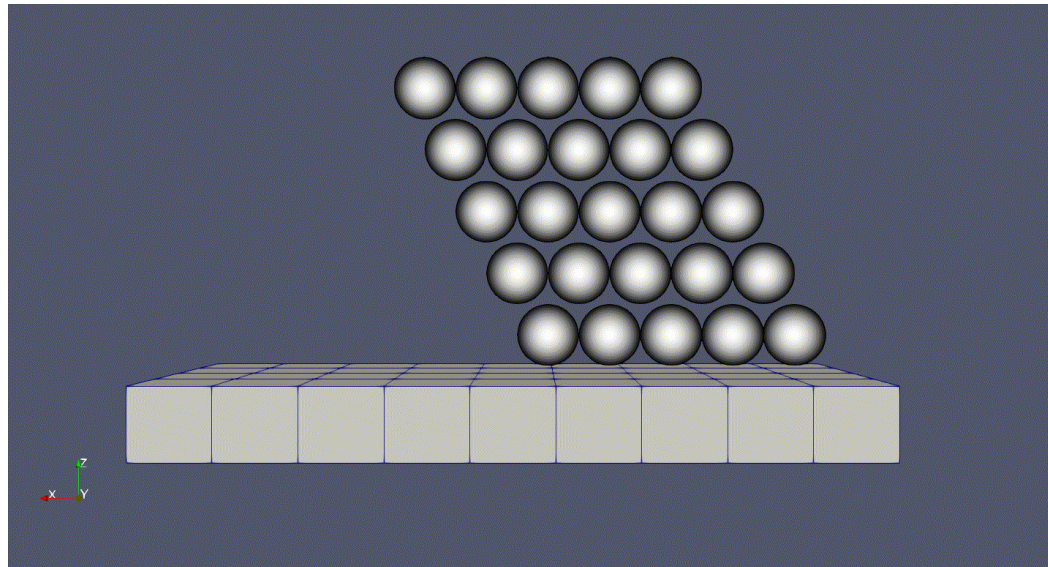




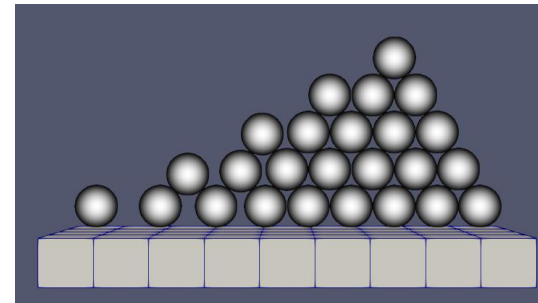
# Spheres assembly collapse

- 25 discrete elements
- Time step  $1 \times 10^{-5} \text{s}$
- Référence: AI, J., CHEN, J., ROTTER, J. & OOI, J. Y., 2011. Assessment of rolling resistance models in discrete element simulations. Powder Technology, 3 206, pp. 269-282.

Variables	Particules	Boîte	Unité
masse volumique	1056	1056	kg/m3
module de Young	$40 \times 10^6$	$40 \times 10^6$	N/m2
coefficient de Poisson	0,49	0,49	-
coefficient de restitution	0,82	-	-
coefficient de friction	0,8	0,8	-
résistance de roulement	0.2	-	-
coefficient d'amortissement	0.6	-	-



EPX result



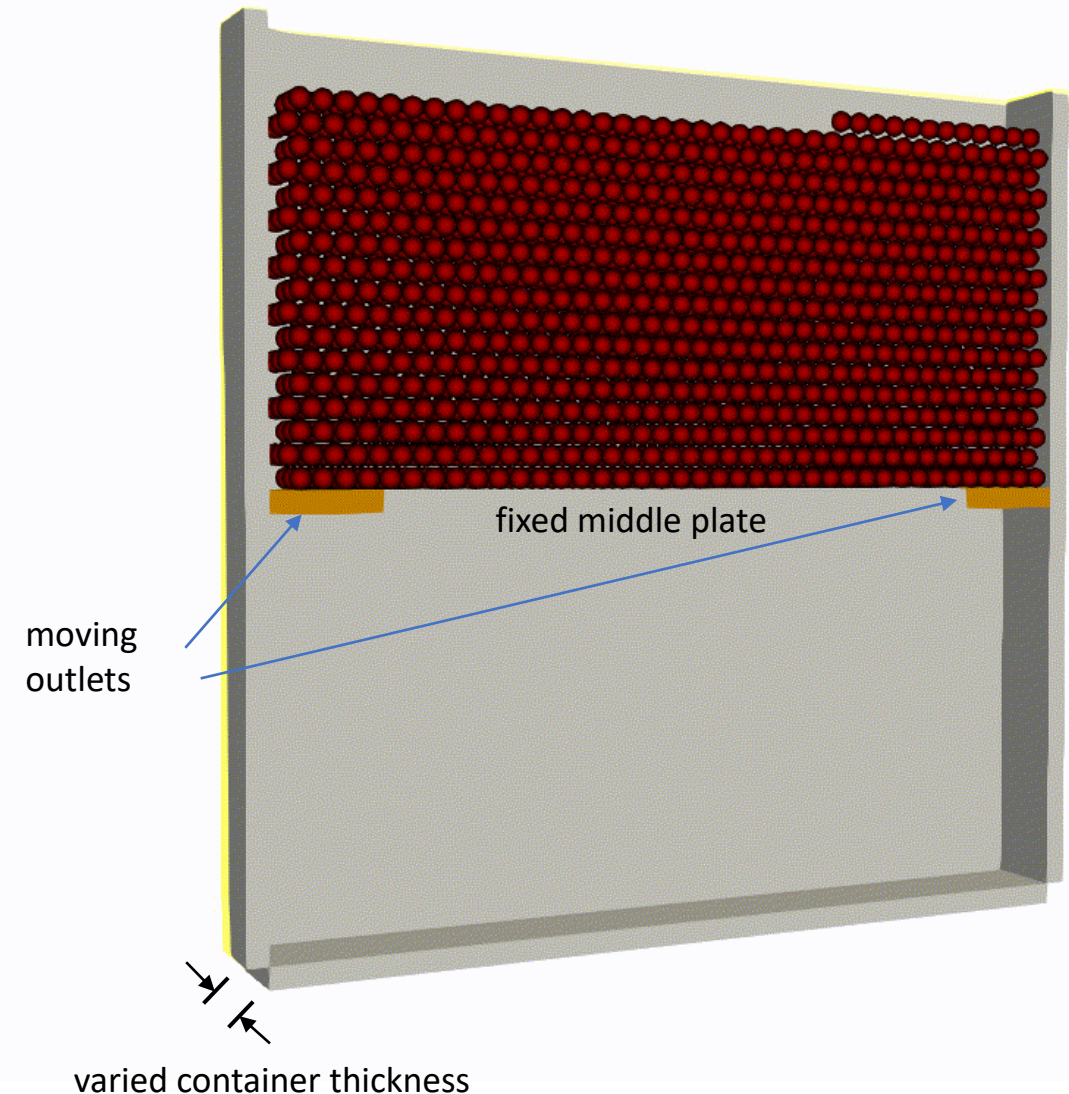
Reference



# Sandpile formation with glass beads

- 2000 particles (2mm)
- Glass particles, wooden container
- Time step  $1 \times 10^{-5} \text{s}$
- Reference : AI, J., CHEN, J., ROTTER, J. & OOI, J. Y., 2011. Assessment of rolling resistance models in discrete element simulations. Powder Technology, 3 206, pp. 269-282.

Paramètres Matériaux			
variables	particules	boîte	unité
masse volumique	2500	2500	kg/m3
module de Young	$2,16 \times 10^6$	$2,16 \times 10^6$	N/m2
coefficient de Poisson	0,3	0,3	-
coefficient de restitution	0,82	-	-
coefficient de frottement	0,3	0,3	-
résistance de roulement	0,05	-	-
coefficient d'amortissement	0.001	-	-
ratio de ks et kn	0,2	-	-

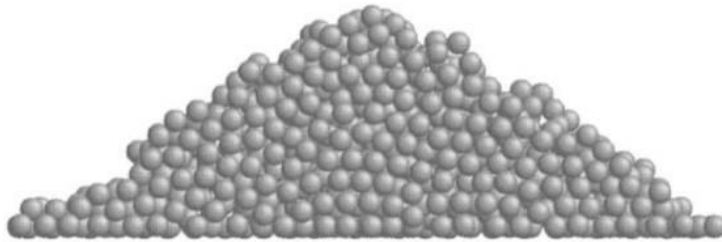


# Sandpile formation with glass beads

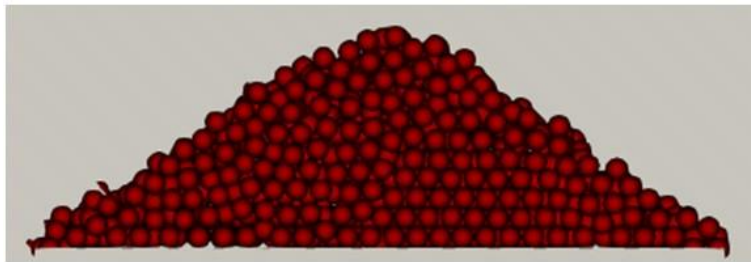
Box thickness =  $4 \times d$



tas final de l'essai ( $33^\circ$ )



tas final de la simulation de Zhou ( $34^\circ$ )

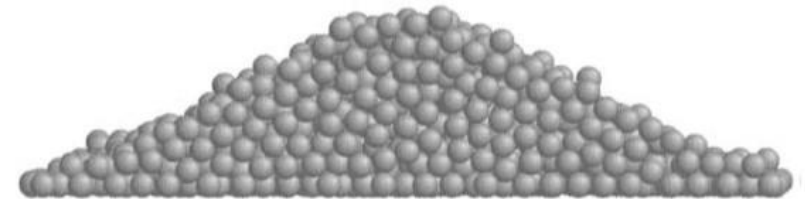


tas final de la simulation EPX ( $34^\circ$ )

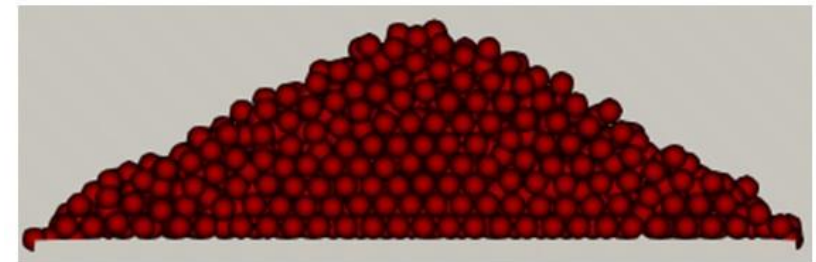
Box thickness =  $20 \times d$



tas final de l'essai ( $26^\circ$ )



tas final de la simulation de Zhou ( $27^\circ$ )



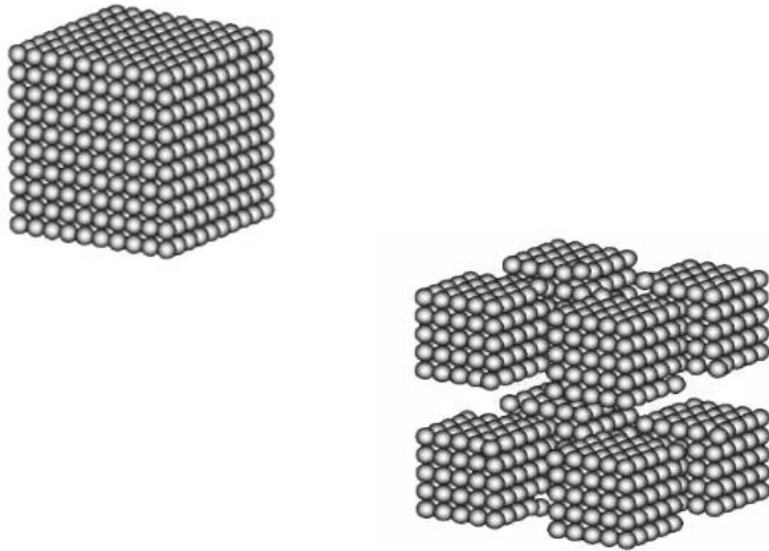
tas final de la simulation EPX ( $29^\circ$ )



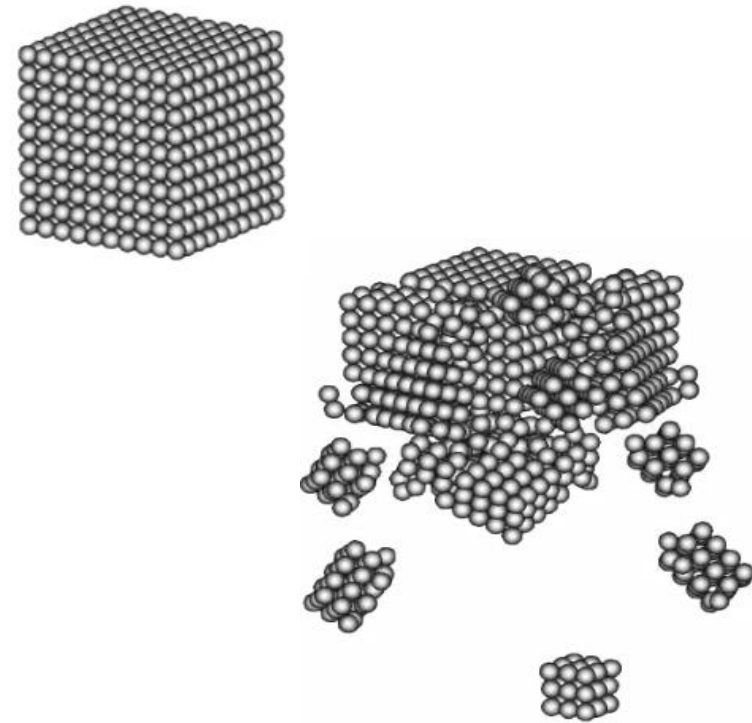
# Fragment break-up

Cube-like fragment composed of 1000 discrete elements glued together by cohesive links

Pressure applied in the center



Off-center pressure



# Modeling relocation and ejection of fuel fragments during LOCA

EDF-LMGC Montpellier thesis

## Physics to model:

- El-pl. swelling of the cladding
- Account for porosity
- Relocation of fragments
- Cladding rupture
- Ejection of fragments in gas flow

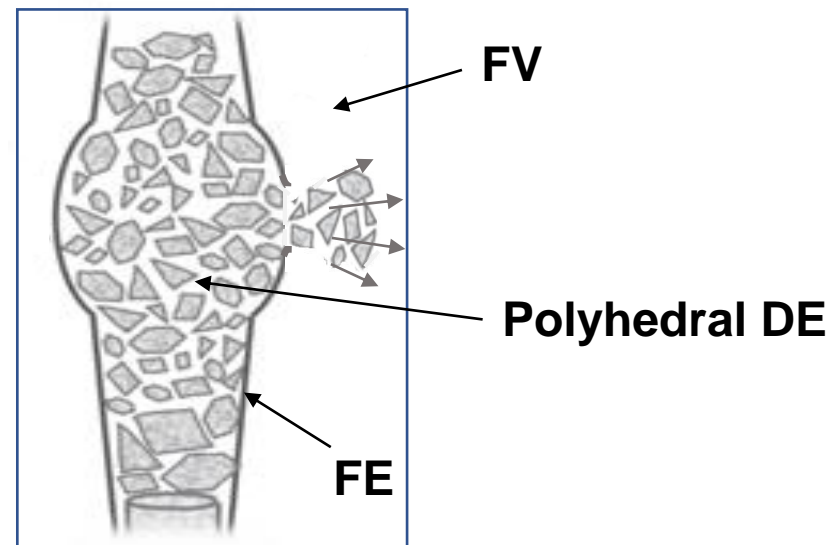


## Expert opinion:

- Size and shape of particles play a crucial role in dynamics of relocation and fragments ejection
- Spherical DE overestimate relocation/ejection
- Additional porosity of spherical DE prevent from obtaining realistic results for DE-fluid coupling

## To be implemented in EPX:

- Polyhedral DE with contact interactions
- DE – FV coupling
- Mixed model: DE + FE + FV + FLSX FSI



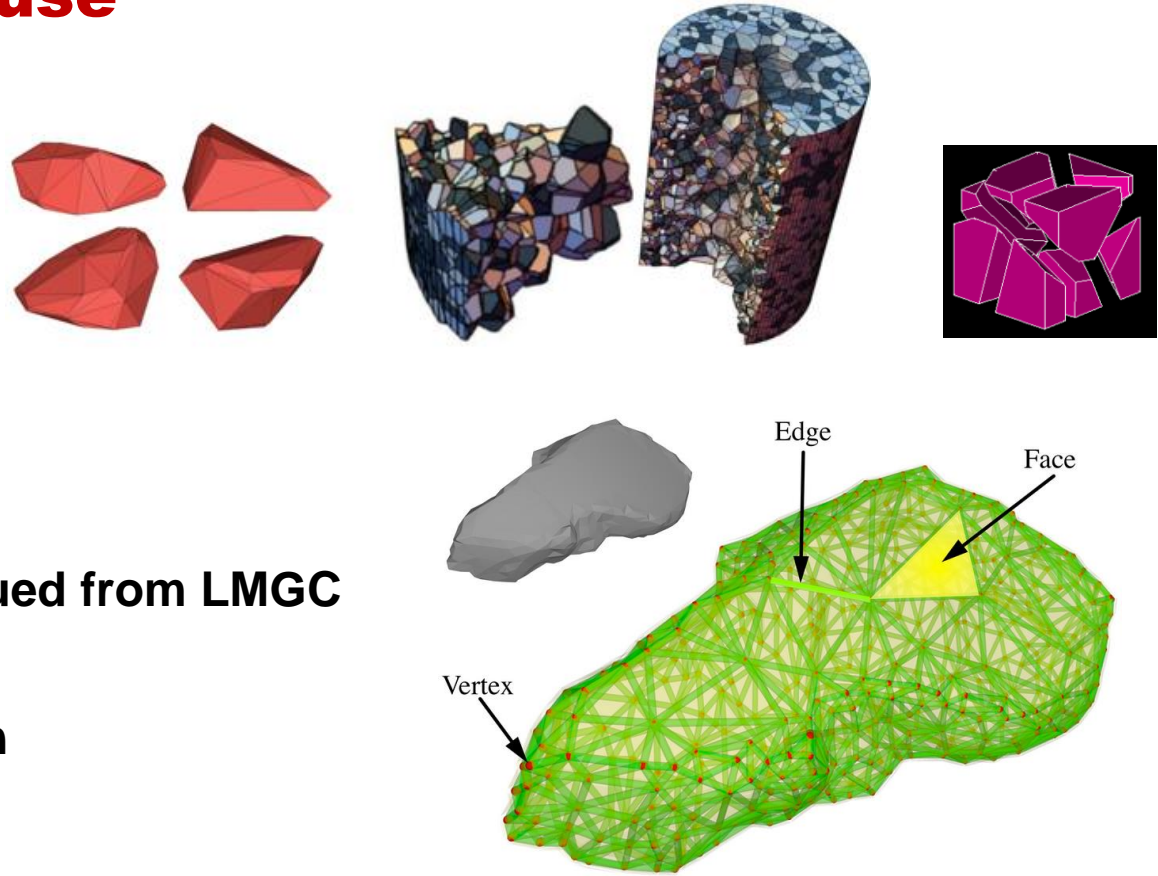
**1<sup>st</sup> year** : Polyhedral DE with contact interactions

**2<sup>nd</sup> year** : DE – fluid interaction: porosity modeling then DE – FV coupling

**3<sup>rd</sup> year**: Interaction of (DE) fragments with elastic-plastic ballooned cladding (FE) and (FV) fluid

# Ingredients to implement/use

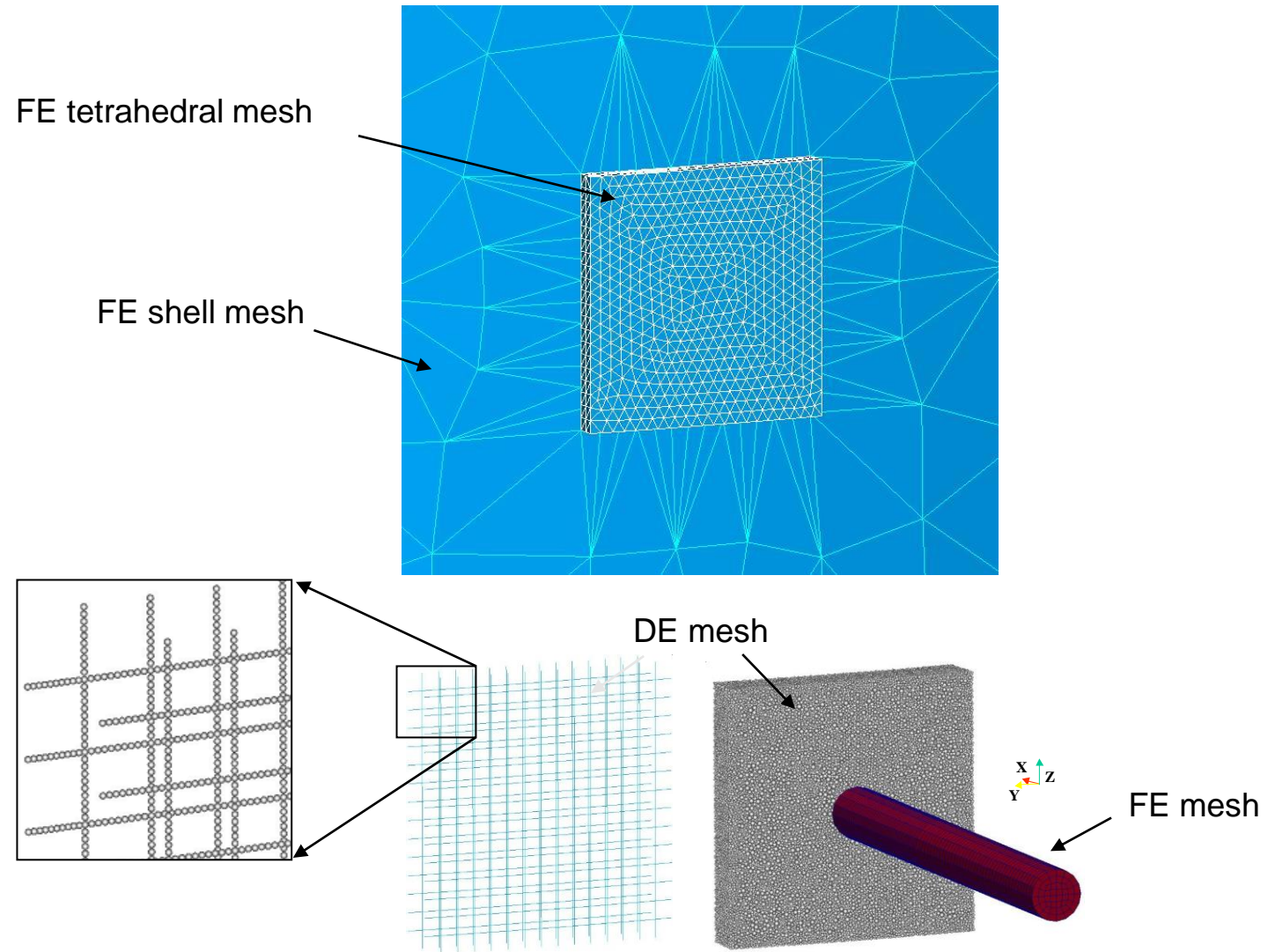
- ❖ MAP tool (EDF) to generate polyhedra
- ❖ Polyhedral mesh in MED format
- ❖ Paraview output in EPX for polyhedra
- ❖ New concept: rigid sphero-polyhedron
- ❖ New technique to manage contacts issued from LMGC Montpellier code Rockable
- ❖ Use of quaternions to define orientation
- ❖ New modules in EPX : `m_eldi_poly.F90`, `m_eldi_poly_liaisons.F90`, ...
  - Motion of 6-dof barycentres
  - Positions of polyhedral's verticies to be deduced to define contact geometry



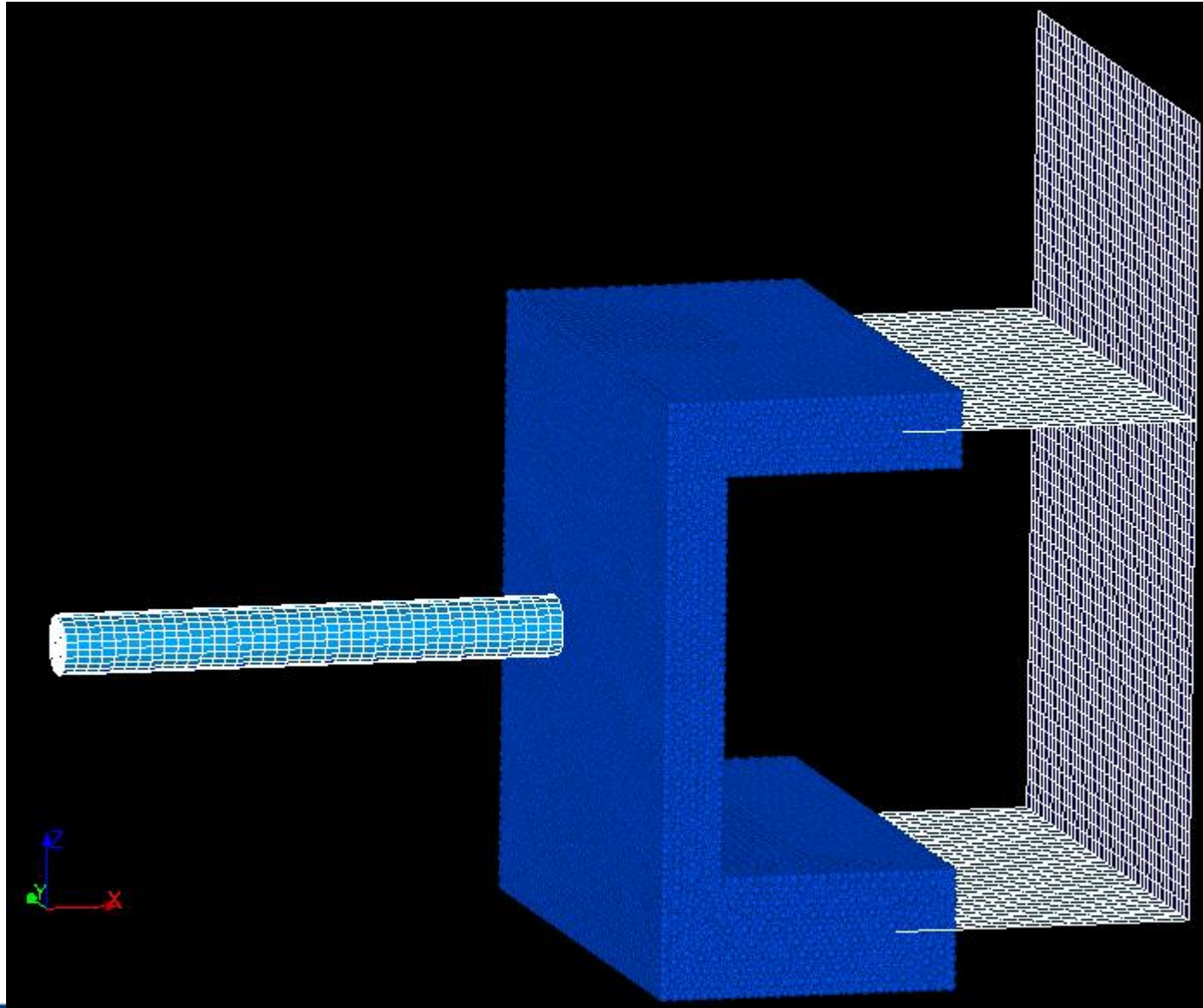


# **Annexes**

# Impact on large RC structures



# Modèles mixtes à géométrie complexe – essai IRIS3

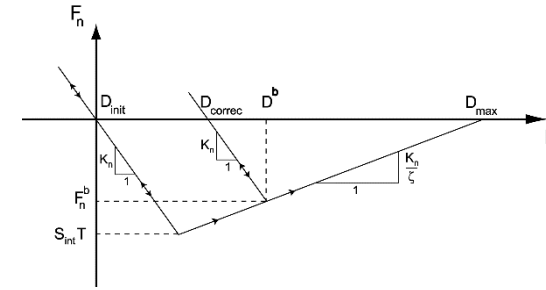
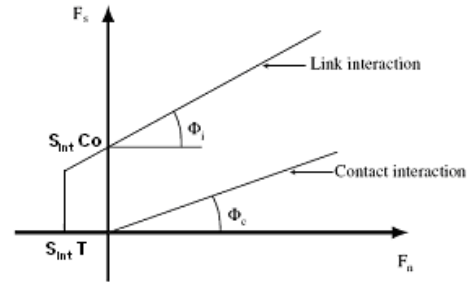


- Géométries non parallélépipédiques avec SpherePadder++
- Plusieurs zones de collage ED-EF coque

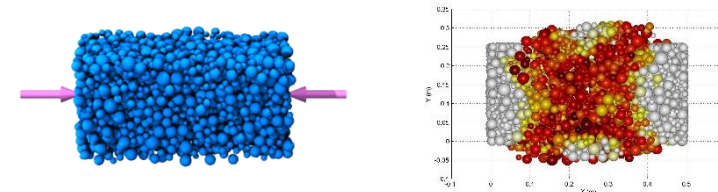
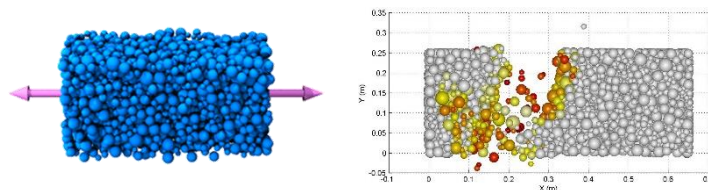
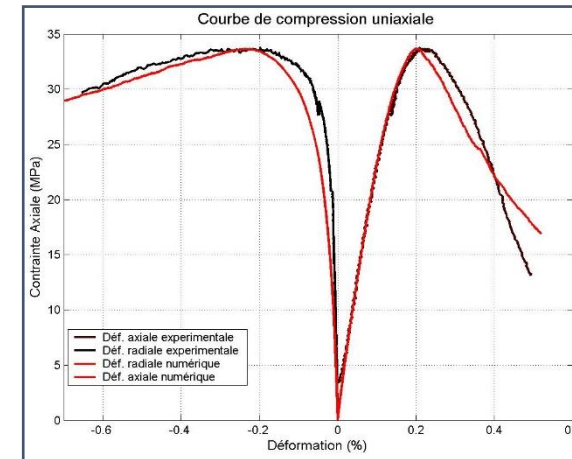
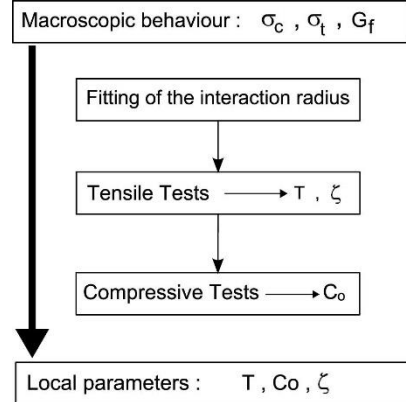
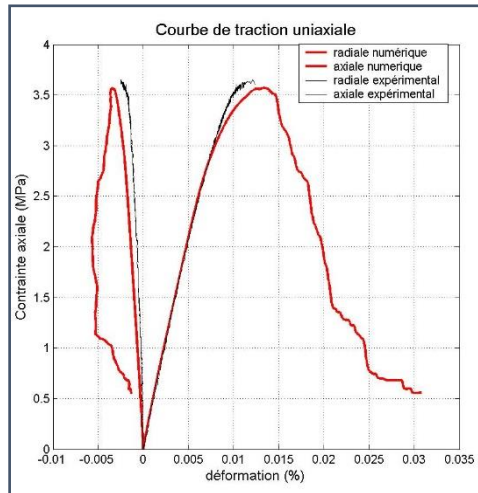


## Brittle behaviour

- cohesive links
- contact behaviour

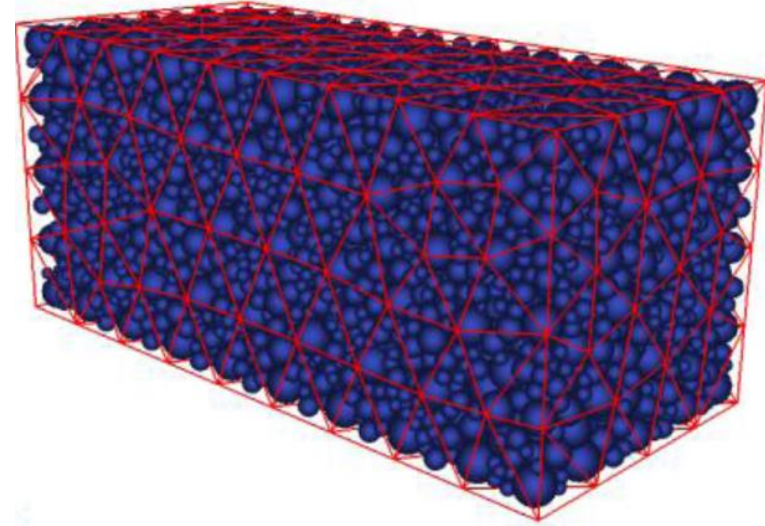


## Identification of $T$ , $\zeta$ , $C_0$ on experimental data



# Discrete Element “mesh”

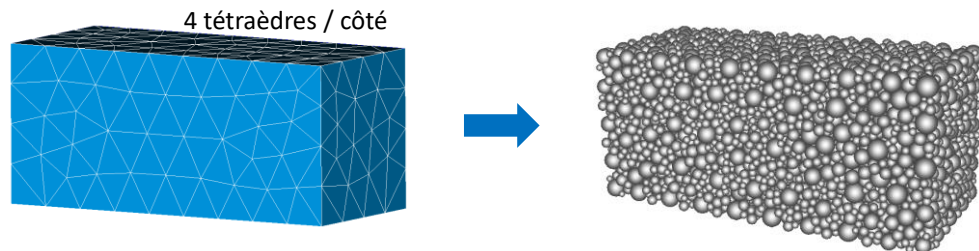
- Tetras-to-DE assembly packing algorithm: Geometric algorithm proposed by Jerier et al. (2009)
- Iterative generation of a mesh with DE of different sizes and masses
- Non-overlapping spheres connected by beam-like interactions
- Typical assumptions to create a homogeneous mesh:
  - $R_{\max}/R_{\min} = 3.0$
  - $FE/DE = 4$
  - Compactness around 0.58



**DE are not constituents of concrete**  
(macroscopic modeling)

# Recalage automatique via Adao du modèle ED

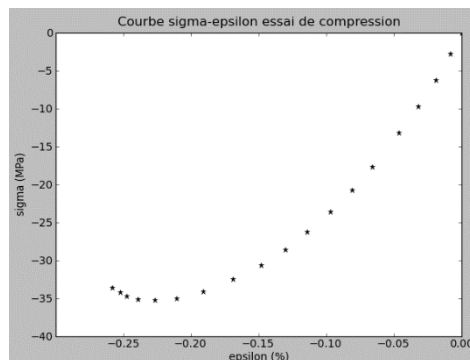
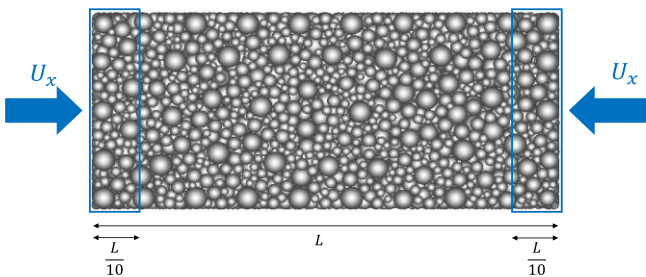
SpherePadder++ (SMESH)



## Identification manuelle des paramètres locaux non-linéaires en 2 étapes :

- on identifie  $\mathbf{T}$  en simulant un essai de traction simple
- on identifie  $\mathbf{C}_0$  en simulant un essai de compression simple

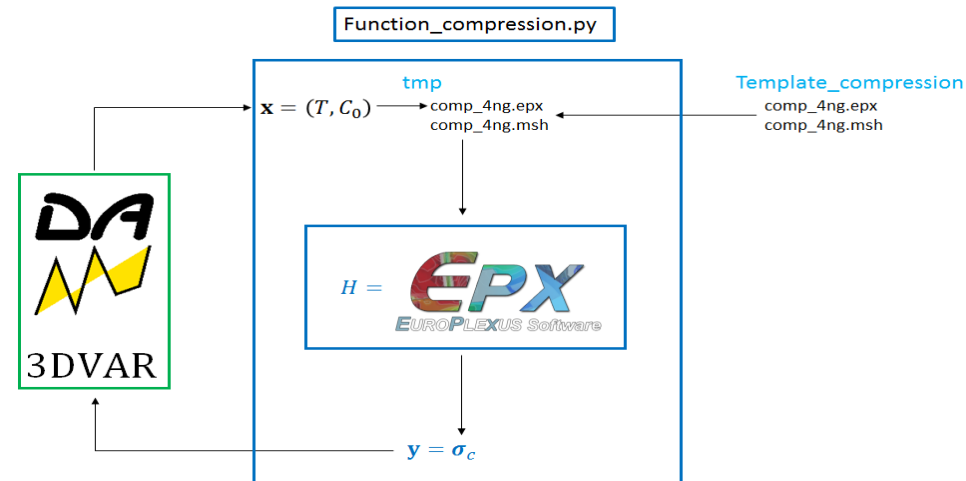
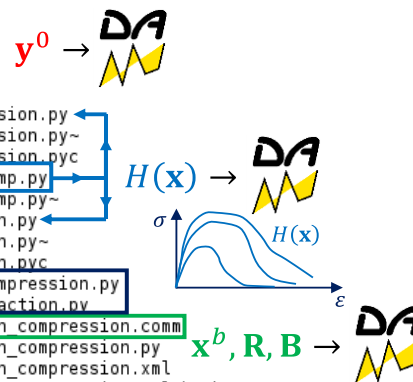
Europlexus



## Identification automatique sous Salome

AM27A62N@aster2:/scratch/AM27A62N/ADAO\_recalage\$ ll

```
total 6400
-rw-r--r-- 1 AM27A62N rdusers 1235 2015-07-28 17:05 fichier_obs.py
-rw-r--r-- 1 AM27A62N rdusers 1188 2015-07-28 17:05 fichier_obs.py~
-rw-r--r-- 1 AM27A62N rdusers 1052 2015-07-28 17:05 fichier_obs.pyc
-rw-r--r-- 1 AM27A62N rdusers 3126 2015-07-28 17:05 function_compression.py
-rw-r--r-- 1 AM27A62N rdusers 3105 2015-07-28 17:05 function_compression.py~
-rw-r--r-- 1 AM27A62N rdusers 2500 2015-07-28 17:05 function_compression.pyc
-rw-r--r-- 1 AM27A62N rdusers 737 2015-07-28 17:05 function_trac_comp.py
-rw-r--r-- 1 AM27A62N rdusers 727 2015-07-28 17:05 function_trac_comp.py~
-rw-r--r-- 1 AM27A62N rdusers 2430 2015-07-28 17:05 function_traction.py
-rw-r--r-- 1 AM27A62N rdusers 2439 2015-07-28 17:05 function_traction.py~
-rw-r--r-- 1 AM27A62N rdusers 2080 2015-07-28 17:05 function_traction.pyc
-rw-r--r-- 1 AM27A62N rdusers 2782 2015-07-28 17:05 print_courbes_compression.py
-rw-r--r-- 1 AM27A62N rdusers 2759 2015-07-28 17:05 print_courbes_traction.py
-rw-r--r-- 1 AM27A62N rdusers 4938 2015-07-28 17:05 recalage_traction_compression.comm
-rw-r--r-- 1 AM27A62N rdusers 4861 2015-07-28 17:05 recalage_traction_compression.py
-rw-r--r-- 1 AM27A62N rdusers 42653 2015-07-28 17:05 recalage_traction_compression.xml
-rw-r--r-- 1 AM27A62N rdusers 42653 2015-07-28 17:05 recalage_traction_compression.xml.back
drwxr-xr-x 2 AM27A62N rdusers 262144 2015-07-28 17:05 template_compression
drwxr-xr-x 2 AM27A62N rdusers 262144 2015-07-28 17:05 template_traction
drwxr-xr-x 137 AM27A62N rdusers 262144 2015-07-28 17:05 tmp = ∅
-rw-r--r-- 1 AM27A62N rdusers 1272858 2015-07-28 17:05 traceExec_proc
```



## Bilan :

- recalage automatique global traction-compression
- algorithme 3DVAR non approprié (Salome 7.6)
- utiliser les algorithmes sans gradient disponibles dans Salome 7.7