

# Is it reasonable to split sand grains before gluing them together?

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## Why a Decomposition Method for granular dynamics ?

### 1. Increasing granular simulation size



Forced-fold evolution on a numerical sandbox : 43 000 grains (2D)

2. DDM may provide a numerical homogenization procedure...  
... if a macroscale description is added for accelerating the convergence.

Is it reasonable to split sand grains before gluing them together?

└ Motivation

└ Domain Decomposition Methods in contact mechanics

# Domain Decomposition Methods in contact mechanics

## 1. Continuum mechanics

- ▶ Balancing Domain Decomposition (BDD)  
[Le Tallec et al 1991] [Mandel 1990]
- ▶ Finite Element Tearing & Interconnecting (FETI)  
[Farhat-Roux 1991]

## 2. Contact mechanics

- ▶ BDD  
[Barboteu-PA 2001] (Newton-Schur)
- ▶ FETI  
[Dureisseix-Farhat 2001] (Projected CG),  
[Dostal et al 1998] (Augmented Lagrangian)

Features : Finite Element context, **Contact on the interfaces**

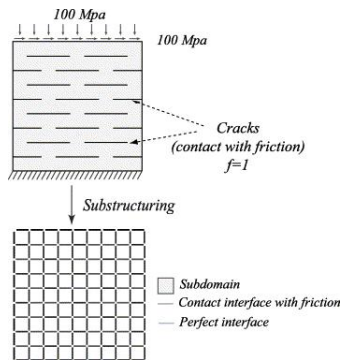
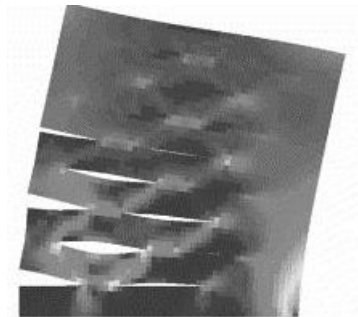
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## Contact generally located on the interfaces

Example of a micro-cracked domain [Ladeveze-Nouy-Loiseau 2002]



- ▶ Non smoothness (contact + friction) dealt with on interfaces.
- ▶ Smooth behavior within the subdomains.

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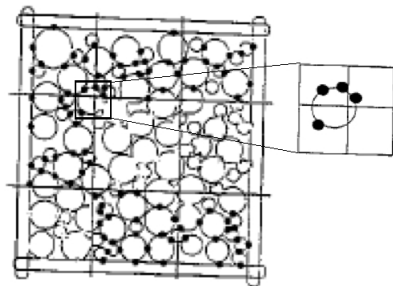
## A pioneering work of the last century

### Modélisation parallèle des matériaux granulaires

Piotr BREITKOPF<sup>1</sup>, Michel JEAN<sup>2</sup>

Distributed memory and message passing [Breitkopf-Jean 1999]

- ▶ Partitioning ("méthode des boîtes") : distributing the contacts
- ▶ Message passing : momentum on the interface grains



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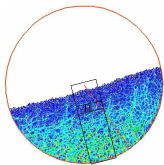
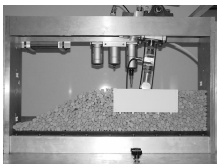
└ Motivation

└ Domain Decomposition Method for granular dynamics

## Domain Decomposition Method for granular dynamics

### Specificities and difficulties of the topic

- ▶ Dynamics of rigid bodies
  - ▶ A velocity/impulse formulation has to be used (next section)
  - ▶ Local dynamics but (often) global statics



- ▶ Discrete system with an evolving connectivity between grains.
  - ▶ How to decompose such a domain ? (further section)
  - ▶ How to update this decomposition ?
- ▶ Non smooth contact dynamics within the whole domain.
  - ▶ The non smoothness cannot be isolated on some interfaces.
  - ▶ No condensation of the equations on the interfaces

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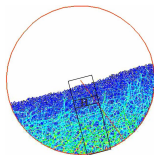
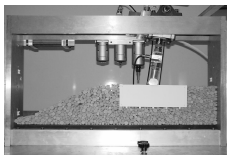
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## Domain Decomposition Method for granular dynamics

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# Outline

## Motivation

Domain Decomposition Methods in contact mechanics

Domain Decomposition Method for granular dynamics

Basic equations and reference problem

Partitioning strategies

Primal partitioning : application to railway ballast

Dual partitioning : theoretical and numerical study

Is it reasonable to split sand grains before gluing them together?

└ Basic equations and reference problem

# Basic equations and reference problem

Motivation

Basic equations and reference problem

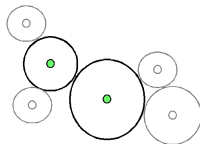
Partitioning strategies

Primal partitioning : application to railway ballast

Dual partitioning : theoretical and numerical study

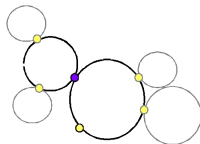
## Granular dynamics with a velocity/impulse formulation

for a grain  $i$



- ▶  $V_i$  : grain velocity
- ▶  $R_i$  : impulse over  $]t^-, t^+]$

for a contact  $\alpha$



- ▶  $v_\alpha$  : relative velocity between 2 grains
- ▶  $r_\alpha$  : contact impulse between 2 grains over  $]t^{--}, t^-]$

## Ingredients

► **Dynamics** (grains)

$$M \dot{V} = M V^- + R^d + R$$

► **Admissibility** equations

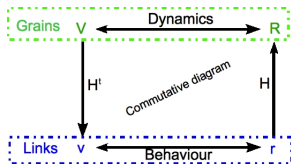
$$v = H^T V$$

$$R = Hr$$

► **Behaviour** (contacts)

$$\mathcal{R}(r_\alpha, v_\alpha) = 0$$

Implicit integration of dynamics  
(differential measures - Moreau 99)



Unilateral contact.

Explicit predictor of the gap  $g_\alpha^p$ .

$$\text{if } g_\alpha^p > 0, \quad r_\alpha = 0$$

$$\text{if } g_\alpha^p \leq 0, \quad 0 \leq r_\alpha \perp v_\alpha \geq 0$$

## Reference problem

- ▶ **(Reduced) dynamics at contacts** (indexed by  $\alpha$ )  
(Dyn) + (Adm) lead to

$$Wr - v = -v^d$$

$W = H^t M^{-1} H$  Delassus operator

$v^d = H^t M^{-1} R^d + H^t V$ , "free" velocity.

- ▶ Reference problem

$$\begin{cases} Wr - v = -v^d \\ \mathcal{R}(r_\alpha, v_\alpha) = 0, \alpha = 1, n_{\text{contact}} \end{cases}$$

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└ Partitioning strategies

# Partitioning strategies

Motivation

Basic equations and reference problem

Partitioning strategies

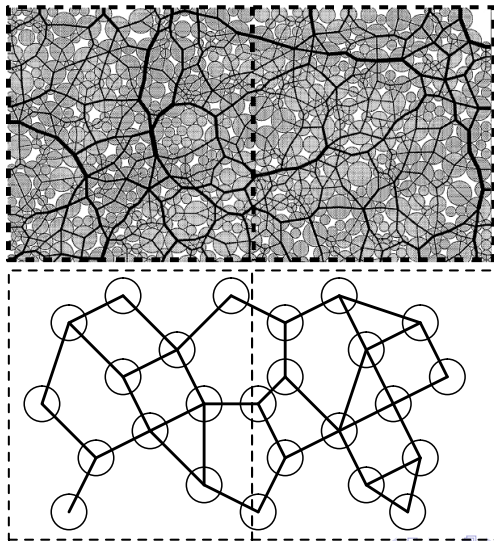
Primal partitioning : application to railway ballast

Dual partitioning : theoretical and numerical study

Is it reasonable to split sand grains before gluing them together?

└ Partitioning strategies

## "Geometrical box" approach for partitioning



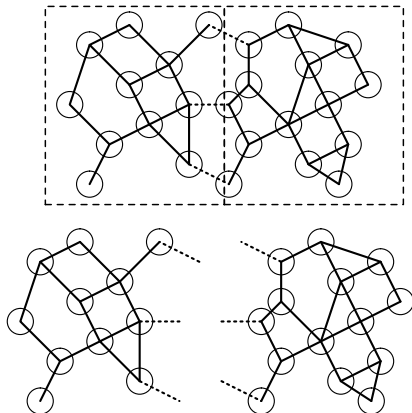
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└ Partitioning strategies

## Primal partitioning

Distributing the **nodes** among substructures

Interfaces = links between substructures



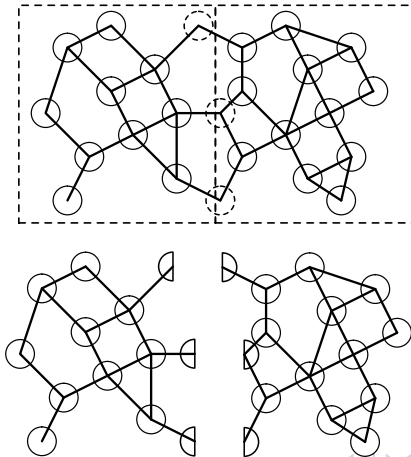
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└ Partitioning strategies

## Dual partitioning

Distributing the **links** among substructures

interfaces = nodes between substructures



Is it reasonable to split sand grains before gluing them together?

└ Primal partitioning : application to railway ballast

# Primal partitioning : application to railway ballast

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## Primal partitioning : **non smooth** interface

Impulsions  $r =$  **internal** (subdomains)  $r_E$  et **interface**  $r_\Gamma$

$$r^t = [\dots, r_E, \dots, r_{E'}, \dots, r_\Gamma]$$

Non smooth problem inside the subdomains  $E...$

$$\begin{cases} W_E r_E - v_E + W_{E\Gamma} r_\Gamma = -v_E^d \\ \mathcal{R}(r_E, v_E) = 0 \end{cases}$$

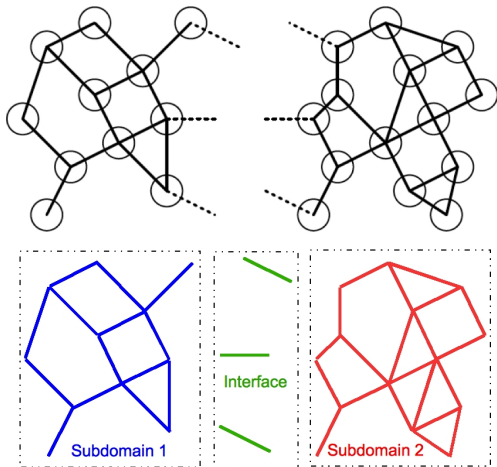
... **and on the interface !**

$$\begin{cases} W_\Gamma r_\Gamma - v_\Gamma - \sum W_{\Gamma E} r_E = -v_\Gamma^d \\ \mathcal{R}(r_\Gamma, v_\Gamma) = 0 \end{cases}$$

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Primal partitioning =  $n + 1$  substructures



Interface with (almost) non connected contacts

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## Reduced dynamics over $n + 1$ subdomains

The linear part is the reduced dynamics

$$\begin{bmatrix} W_E & 0 & W_{E\Gamma} \\ 0 & W_{E'} & W_{E'\Gamma} \\ W_{\Gamma E} & W_{\Gamma E'} & W_{\Gamma} \end{bmatrix} \begin{bmatrix} r_E \\ r_{E'} \\ r_{\Gamma} \end{bmatrix} - \begin{bmatrix} v_E \\ v_{E'} \\ v_{\Gamma} \end{bmatrix} = - \begin{bmatrix} v_E^d \\ v_{E'}^d \\ v_{\Gamma}^d \end{bmatrix}$$

Properties

- ▶ The problems per subdomains are uncoupled
- ▶  $W_{\Gamma}$  is quasi-diagonal.

## Gauss-Seidel like algorithm (with a particular renumbering)

- ▶ **Step 1** : GSNL solution per subdomain (parallel computing)

Gauss-Seidel like partitioning per block

$W_E^L$  = diagonal and lower triangular parts of  $W_E$

$$(W_E = W_E^L + (W_E - W_E^L)).$$

$$\begin{cases} W_E^L r_E^k - v_E^k = -v_E^d - W_{E\Gamma} r_\Gamma - (W_E - W_E^L) r_E^{k-1} \\ \mathcal{R}(r_E^k, v_E^k) = 0 \end{cases}$$

$k$  = number of Gauss-Seidel sweeps.

- ▶ **Step 2** : GSNL solution at the interface

$$\begin{cases} W_\Gamma^L r_\Gamma^k - v_\Gamma^k = -v_\Gamma^d - \sum W_{\Gamma E} r_E - (W_\Gamma - W_\Gamma^L) r_\Gamma^{k-1} \\ \mathcal{R}(r_\Gamma^k, v_\Gamma^k) = 0 \end{cases}$$

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└ Primal partitioning : application to railway ballast

└ Railway ballast topic

Motivation

Basic equations and reference problem

Partitioning strategies

**Primal partitioning : application to railway ballast**  
Railway ballast topic

Dual partitioning : theoretical and numerical study

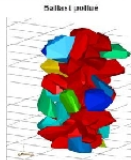
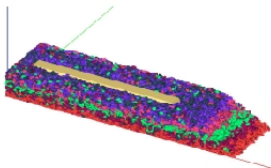
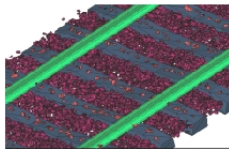
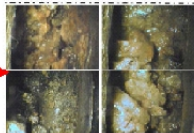
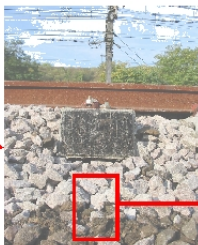
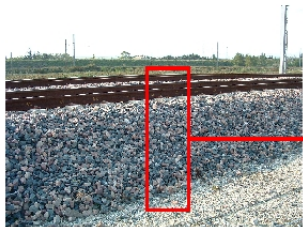
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## Railway ballast topic

Complex medium - Polyhedral grains - Relevant discrete scale



Is it reasonable to split sand grains before gluing them together?

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## Identification of relevant parameters

Evolutionary nonsmooth problem  $\Rightarrow$  **solution multiplicity**

$\Rightarrow$  a set of qualitative **indicators** to qualify the computations

- ▶ **Volume error** (quantifying interpenetration)
- ▶ Compactness
- ▶ **Coordination number** (average neighbors number)
- ▶ Simple / double / triple contacts number
- ▶ Average / maximum velocity magnitude
- ▶ Inertia parameter

$$I = \dot{\epsilon} \sqrt{\frac{m}{p \cdot d}}$$

$\dot{\epsilon}$  : shear velocity

$m$  : average grain mass.

$p$  : average pressure.

$d$  : average grain diameter.

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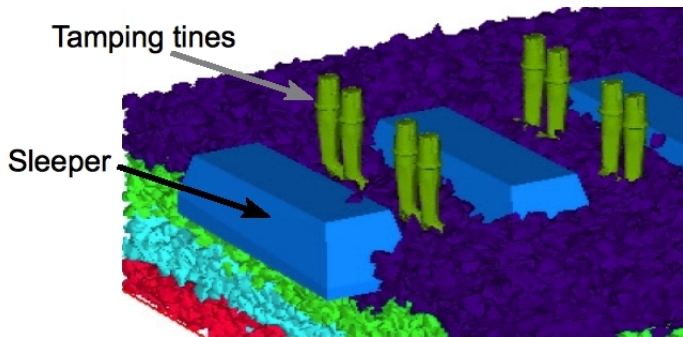
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└ Railway ballast topic

## A maintenance example : the tamping process

Three phases (with vibrating forces and after lifting of the sleeper)

- ▶ Penetration of the tamping tines
- ▶ Squeezing of the ballast grains under the sleeper
- ▶ Lifting the tamping tines



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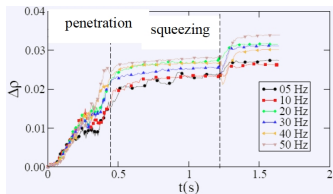
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## Example of a parametric study on a single sleeper

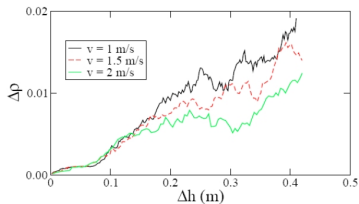
[Saussine et al., WCRR 2008]

- ▶ Evolution of the compaction under the sleeper



Penetration phase contributes to 50% of the final compaction gain

- ▶ The compaction with respect to the driven velocity



Low speeds improve the final compaction gain

→ Recommendation

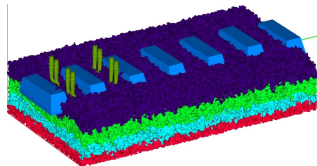
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## Penetration phase on a long railway slice :

90 000 grains, 310 000 contacts,  
7 subdomains, 1 interface



	Sleeper 1	Sleeper 2	Sleeper 3	Sleeper 4	Sleeper 5	Sleeper 6	Sleeper 7
R	800	800	800	800	800	800	800
1	800	800	800	700	700	700	700
2	800	800	800	700	600	500	400
3	800	800	800	700	500	300	200
4	800	800	800	100	200	300	400

Number of sweepings for each SD in 5 runs  
(Reference and 4 cases with different # sweepings per SD)

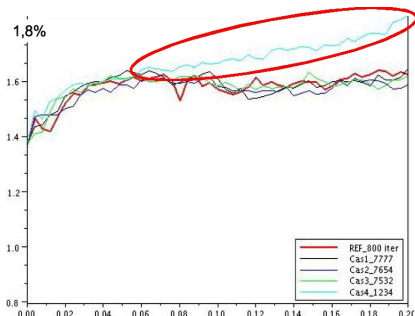
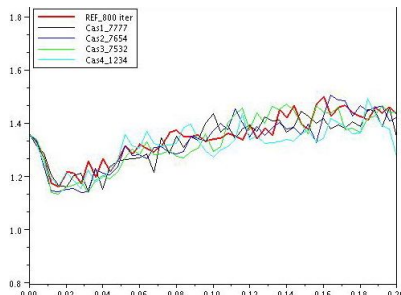
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## Comparison of the volume (interpenetration) error ( $< 2\%$ )

Sleeper 3 / Sleeper 4



100 sweepings (run 4) for SD4 is not sufficient to avoid interpenetration...  
but the error does not propagate to others SD.

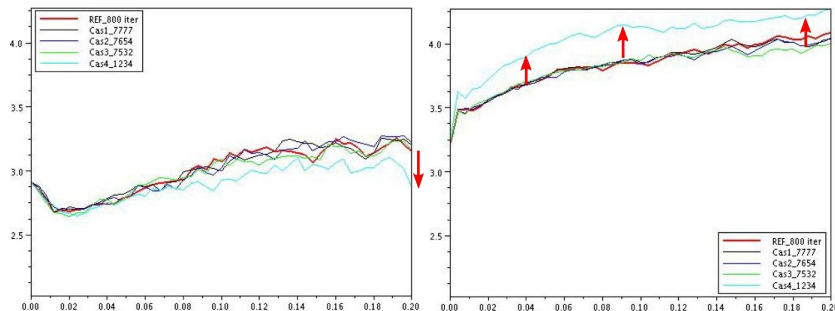
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## Comparison of the coordination number ( $\approx$ compactness )

Sleeper 3 / Sleeper 4



100 sweepings (run 4) for SD4 overestimates the coordination number...  
and underestimates it on the neighboring SD3!

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## First conclusions and forthcoming works

- ▶ Easy to implement (simple renumbering)
- ▶ Developing parallel versions with OpenMP (then MPI?)
- ▶ Defining forerunner indicators of dynamic behaviour

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└ Dual partitioning : theoretical and numerical study

## Dual partitioning : theoretical and numerical study

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Primal partitioning : application to railway ballast

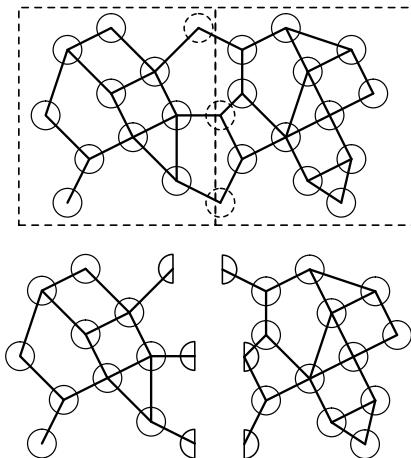
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## Dual partitioning : distributing the **links** among substructures

**non smooth** subdomains... but **perfect** interface



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## System to solve

**Non smoothness** within the subdomains

$$\left\{ \begin{array}{l} W_E r_E - v_E - H_E^t M_E^{-1} A_{E\Gamma}^t F_\Gamma = -v_E^d \\ \mathcal{R}(v_E, r_E) = 0 \end{array} \right\} E = 1, \dots, n_{SD}$$

**Perfect** velocity continuity at the interfaces (between half-grains)

$$\sum_E A_{E\Gamma} V_E = 0$$

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## FETI type formulation

Rewriting the last equation with the Lagrange multiplier  $F_\Gamma$

$$\left\{ \begin{array}{l} W_E r_E - v_E - H_E^t M_E^{-1} A_{E\Gamma}^t F_\Gamma = -v_E^d \\ \mathcal{R}(v_E, r_E) = 0 \end{array} \right\} E = 1, \dots, n_{SD}$$
$$X F_\Gamma - \sum_E A_{E\Gamma} M_E^{-1} R_E = \sum_E A_{E\Gamma} M_E^{-1} R_E^d$$

with

$$X = \sum_E A_{E\Gamma} M_E^{-1} A_{E\Gamma}^t.$$

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└ A first NLGS-DD solver

## A first NLGS-DD solver

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An enriched algorithm (work in progress)

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## A first NLGS-DD algorithm

- ▶ **Step 1** :  $(\bar{r}_E, \bar{F}_\Gamma)$  known, determining  $(r_E, v_E), \forall E$   
Non Linear Gauss-Seidel algorithm per subdomain  
(possibly incomplete resolution)

$$\begin{cases} W_E r_E - v_E = H_E^t M_E^{-1} A_{E\Gamma}^t \bar{F}_\Gamma - v_E^d \\ \mathcal{R}(v_E, r_E) = 0 \end{cases}$$

- ▶ **Step 2** : Updating of the interface forces  $F_\Gamma$ ,

$$X F_\Gamma = \sum_E A_{E\Gamma} M_E^{-1} (R_E + R_E^d)$$

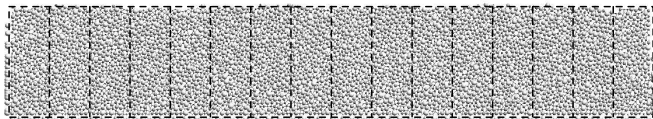
**X diagonal !**

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## Results for a network of 5191 particles and 10177 interactions



Three studied cases

- ▶ Linear interactions :  $\mathcal{R}(v, r) = 0 \leftrightarrow r = -\frac{1}{\epsilon} v$  ("elastic" truss)
  - ▶  $\epsilon = \epsilon_0$  where  $\frac{1}{\epsilon_0}$  is the mean value of the diagonal part of  $W$
  - ▶  $\epsilon = \epsilon_1 = 0.02 \epsilon_0$  (more rigid links)
- ▶ Non smooth interactions : frictionless contact

$$0 \leq r_\alpha \perp v_\alpha \geq 0$$

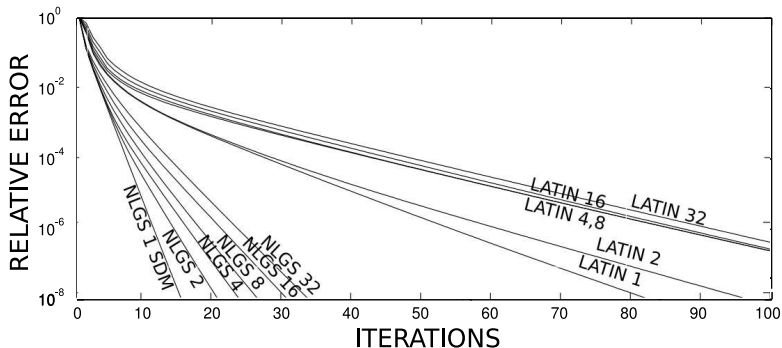
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## Convergence / subdomain number

$\epsilon = \epsilon_0$  where  $\frac{1}{\epsilon_0}$  is the mean value of the diagonal part of  $W$



NON SCALABLE

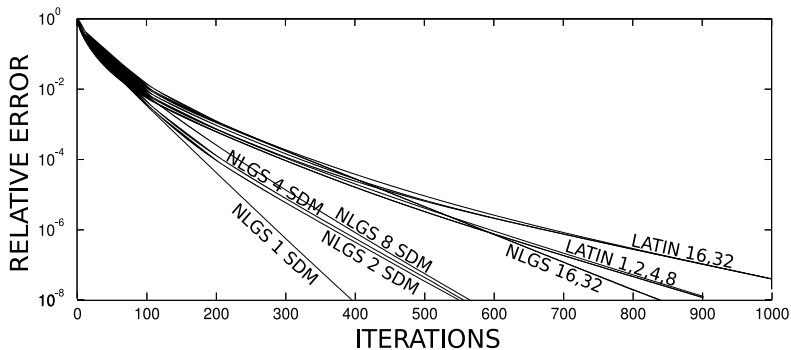
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## Convergence / subdomain number

$\epsilon = \epsilon_1 = 0.02 \epsilon_0$  (more rigid links)



SCALABLE? (quantum scalable?)

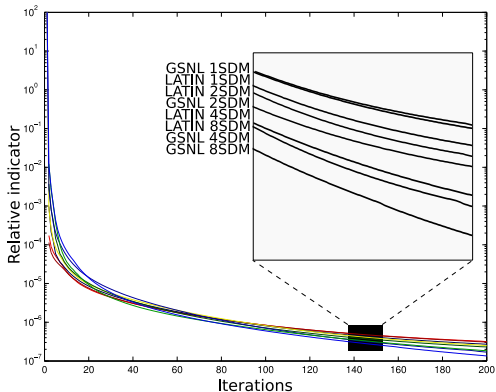
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## Convergence / subdomain number

Non smooth interactions : frictionless contact



SCALABLE... BUT SLOW

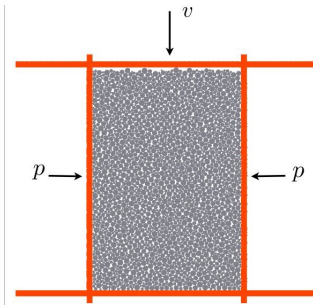
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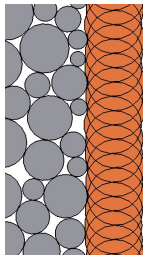
└ A first NLGS-DD solver

## Influence of the decomposition on the solution

### Biaxial test



- ▶ 2 400 particles
- ▶  $\mu = 0.5$
- ▶ Deformable membrane
- ▶ Quasi-static regime (Gdr MiDi 2004)



$$I = \dot{\epsilon} \sqrt{\frac{m}{p}} \ll 1$$

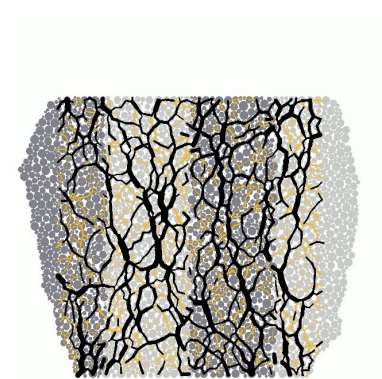
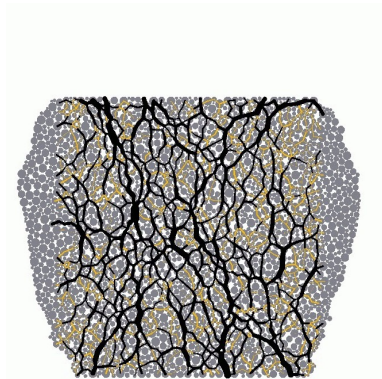
Decompositions :



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└ Dual partitioning : theoretical and numerical study

└ A first NLGS-DD solver



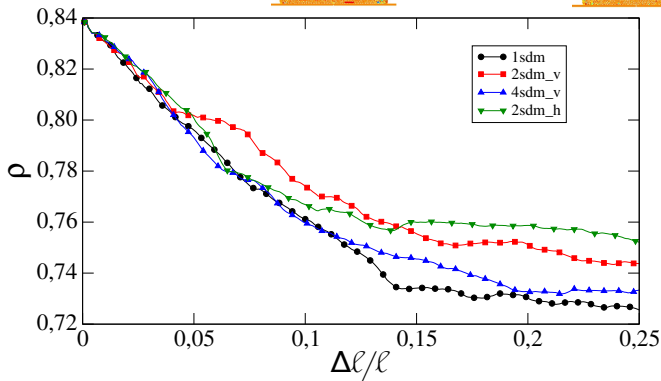
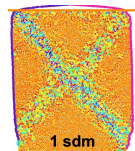
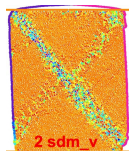
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## Macro behaviour : compactness

$$\rho = \frac{\sum V_p}{V}$$



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## First conclusions

### ▶ Advantages

- ▶ No convergence degradation of the nonsmooth DDM solver
- ▶ Easy to implement (second step = updating)

### ▶ Drawbacks

- ▶ No improvement of the convergence with a macro procedure (X diagonal)
- ▶ No coupling between the interfaces of a subdomain (X diagonal)

⇒ enriching the interface problem

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└ An enriched algorithm (work in progress)

## An enriched algorithm (work in progress)

Motivation

Basic equations and reference problem

Partitioning strategies

Primal partitioning : application to railway ballast

Dual partitioning : theoretical and numerical study

A first NLGS-DD solver

An enriched algorithm (work in progress)

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## An enriched algorithm (work in progress)

The equations (reminder)

▶ Dynamics :  $M_E V_E - R_E + A_{E\Gamma}^t F_\Gamma = F_E^d$ ,  $E = 1, n_{SD}$  (Dyn)

▶ Admissibility :  $v_E = H_E^t V_E$  and  $R_E = H_E r_E$  (Adm)

▶ **Behaviour** :  $\mathcal{R}(r_E, v_E) = 0$  (**nonsmooth !**) (**Beh**)

▶ Interface :  $\sum_E A_{E\Gamma} V_E = 0$  (Int)

Combination for the step 2 of the previous generic algorithm

▶ (Dyn) + (Adm) + (Int)  $\Rightarrow X F_\Gamma = \sum_E A_{E\Gamma} M_E^{-1} (R_E + R_E^d)$

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## Enriching the equation (2)

- ▶ Intermediate variables :  $(\tilde{r}_E, \tilde{v}_E)$  satisfying...
- ▶ ...a "numerical tangent linear behaviour" (search direction)

$$(\tilde{r}_E - r_E) + \frac{1}{\eta}(\tilde{v}_E - v_E) = 0 \quad (\text{Dir})$$

- ▶ Combining (Dyn)+(Adm)+(Int)+(Dir), (2) is replaced by

$$X_\eta F_\Gamma = \sum_E A_{E\Gamma} M_{\eta,E}^{-1} [R_E^d + H_E(r_E + \frac{1}{\eta} v_E)]$$

$$X_\eta = \sum_E A_{E\Gamma} M_{E,\eta}^{-1} A_{E\Gamma}^t \quad \text{and} \quad M_{E,\eta} = M_E + \frac{1}{\eta} \underbrace{H_E H_E^t}_{\text{stiffness like}}$$

$$\text{to compare with } X = \sum_E A_{E\Gamma} M_E^{-1} A_{E\Gamma}^t$$

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## The enriched algorithm

$(\bar{r}_E, \bar{v}_E, \bar{F}_\Gamma)$  known,

► **Step 1** : Determining  $(r_E, v_E), \forall E,$

$$\begin{cases} W_E r_E - v_E = H_E^t M_E^{-1} (A_{E\Gamma}^t \bar{F}_\Gamma - R_E^d) \\ \mathcal{R}(v_E, r_E) = 0 \end{cases}$$

► **Step 2** : Solving the following system to determine  $F_\Gamma,$

$$X_\eta F_\Gamma = \sum_E A_{E\Gamma} M_{\eta,E}^{-1} [R_E^d + H_E (r_E + \frac{1}{\eta} v_E)]$$

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## Interpretation for a linear problem

Linear behaviour law :  $\mathcal{R}(v_E, r_E) = 0 \iff r_E = -\frac{1}{\epsilon} v_E$

- ▶ **Step 1** : Determining  $r_E, \forall E$  ( $v_E$  is eliminated),

$$(W_E + \epsilon I_d) r_E = H_E^t M_E^{-1} (A_{E\Gamma}^t \bar{F}_\Gamma - R_E^d)$$

- ▶ **Step 2** : Solving the following system to determine  $F_\Gamma$ ,

$$X_\eta F_\Gamma = \sum_E A_{E\Gamma} M_{E,\eta}^{-1} [R_E^d + H_E \underbrace{\left(1 - \frac{\epsilon}{\eta}\right)}_{=0 \text{ if } \eta=\epsilon} r_E]$$

If  $\eta = \epsilon$

- ▶ Step 2 does not depend on Step 1  
(convergence with a single iteration)
- ▶ Step 2 is the complete interface problem of the linear global one,

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## An analytical/numerical study...

Linear case  $\Rightarrow$  fixed point mapping  $T_\Gamma : \bar{F}_\Gamma \rightarrow F_\Gamma$

► Generic algorithm :  $T_\Gamma(\bar{F}_\Gamma) = \underbrace{X^{-1}Y_\epsilon}_{B_\epsilon} \bar{F}_\Gamma$

$B_\epsilon$  : contraction matrix

► Enriched version :  $T_\Gamma(\bar{F}_\Gamma) = \underbrace{X_\eta^{-1}Y_{\epsilon,\eta}}_{B_{\epsilon,\eta}} \bar{F}_\Gamma$

$B_{\epsilon,\eta}$  : contraction matrix

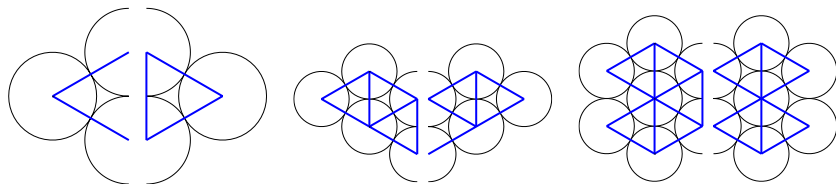
... via 3 small examples ...

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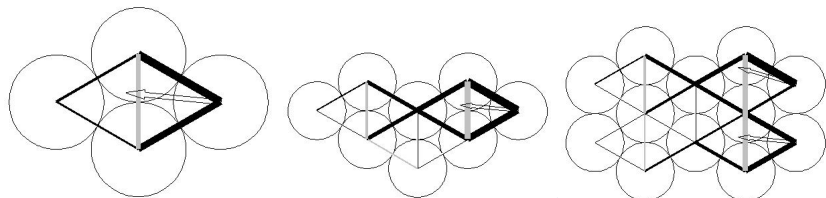
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... via 3 small examples using MAPLE



Contacts or links (matrices  $H_E$ ,  $E = 1, 2$ ) in blue for 4, 8 and 12 disks

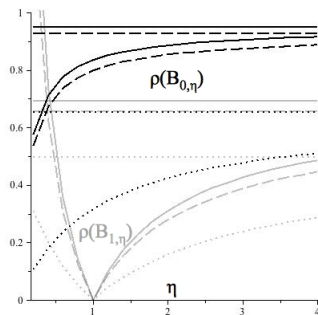
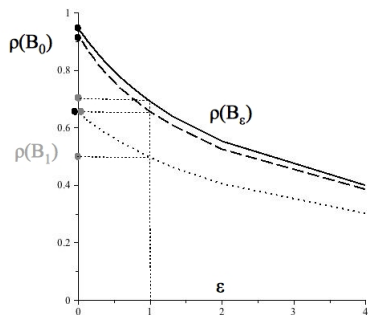


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## Spectral radius of the contraction matrix (linear case)



- ▶ Convergence rate degradation when  $\epsilon \rightarrow 0$  (rigid case)
- ▶ Non reachable optimal convergence when  $\epsilon = 0$  and  $\eta \rightarrow 0$ ...
- ▶ ... except to consider the limit problem with an asymptotic study (out of purpose).

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## Asymptotic convergence for a nonsmooth case

Nonsmooth case (unilateral condition)  $\Rightarrow$  study close to the solution characterized by the **active contacts** defining  $\bar{H}_E$  ( $\bar{H}_E \neq H_E$ , **potential contacts**)

► Generic algorithm :  $T_\Gamma(\bar{F}_\Gamma) = \underbrace{X^{-1}\bar{Y}}_{\bar{B}} \bar{F}_\Gamma$

where  $\bar{Y} = Y_0$  with  $\bar{H}_E$  instead of  $H_E$

► Enriched version :  $T_\Gamma(\bar{F}_\Gamma) = \underbrace{X_\eta^{-1}\bar{Y}_\eta}_{\bar{B}_\eta} \bar{F}_\Gamma$

where  $\bar{Y}_\eta$  mixes  $\bar{H}_E$  and  $H_E$

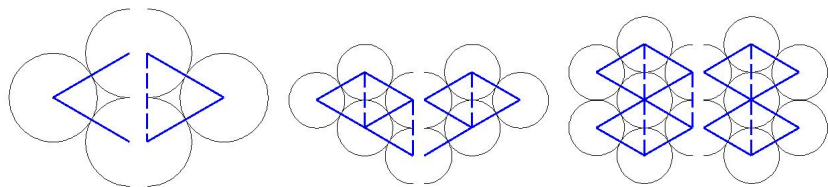
... via 3 small examples ...

Is it reasonable to split sand grains before gluing them together?

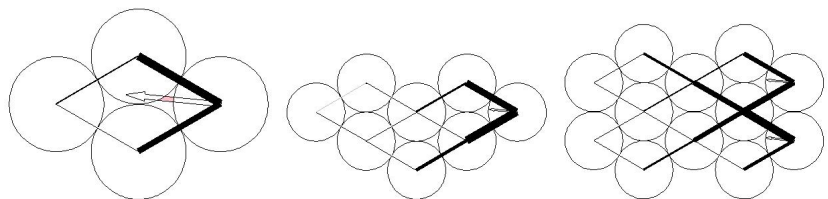
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... via 3 small examples using MAPLE



Active contacts (solid lines,  $\bar{H}_E$ ), Potential contacts (solid & dash lines,  $H_E$ ),

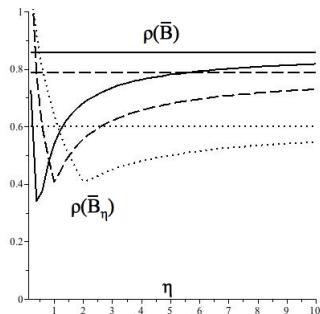


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## Spectral radius of the contraction matrix (nonsmooth case)



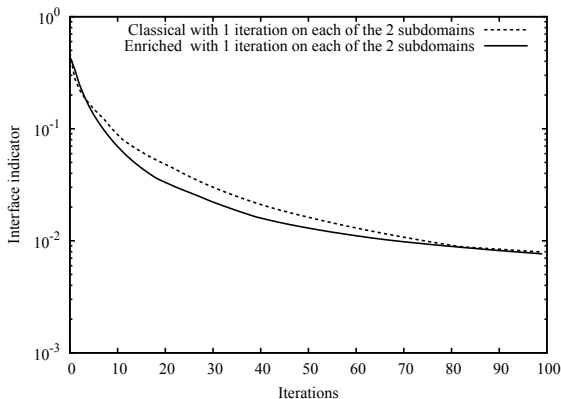
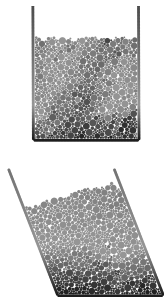
- ▶ Using  $\eta = 0$  seems to be excluded.
- ▶ Optimal range of  $\eta$  ↘ drastically when contact number ↗.  
Finding a good  $\eta$  for a more general case is a challenge!
- ▶ + partial asymptotic theoretical results (not presented)

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... via larger test using LMGC90

Shear test with  
friction and 1000  
disks



A very weak improvement of the convergence!

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## By way of conclusion

- ▶ A lot of open questions
- ▶ A lot of work to propose, analyze and implement an efficient DDM in a granular dynamics software
- ▶ But is it quite reasonable considering the potential gains ?