Contacts: Numerical schemes based on convex optimization problems

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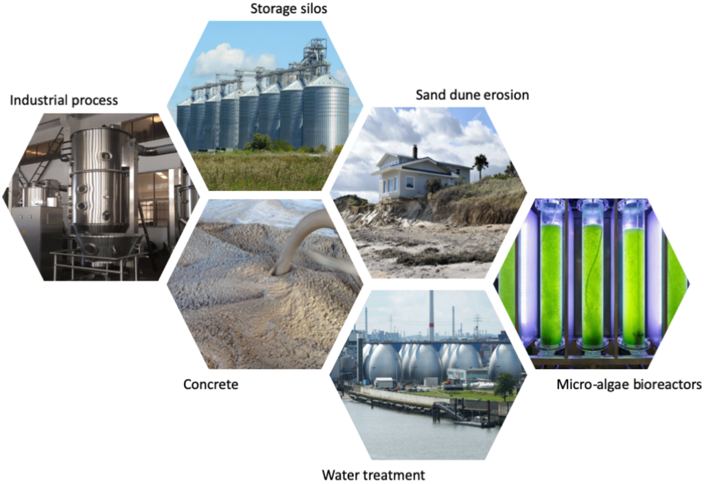
ANR
RheoSuNN

Why study granular media?



Rheology

Objective : Study of the deformation and flow of matter under the effect of an applied stress

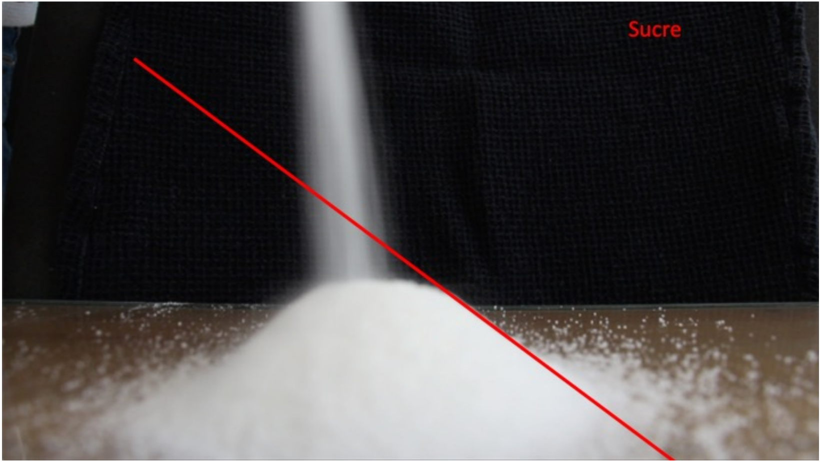
- flow, segregation, mixing, blocking, collapse...

Macroscopic behaviour

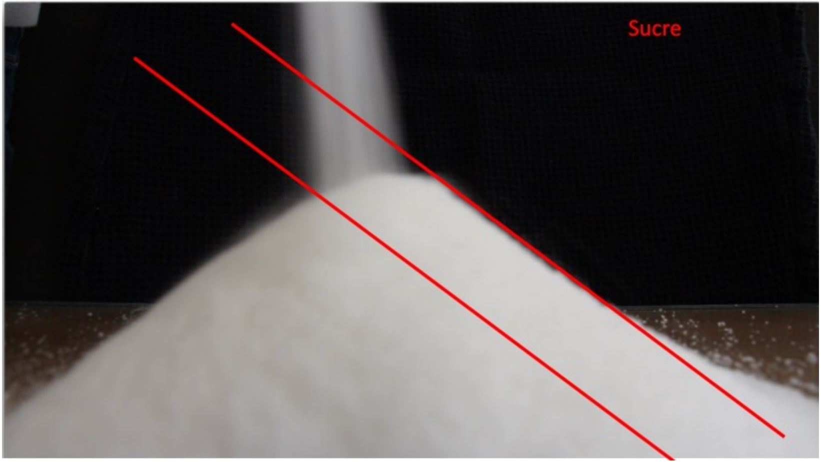
$\Longrightarrow$ Still not well understood

$\Longrightarrow$ Active domain of research

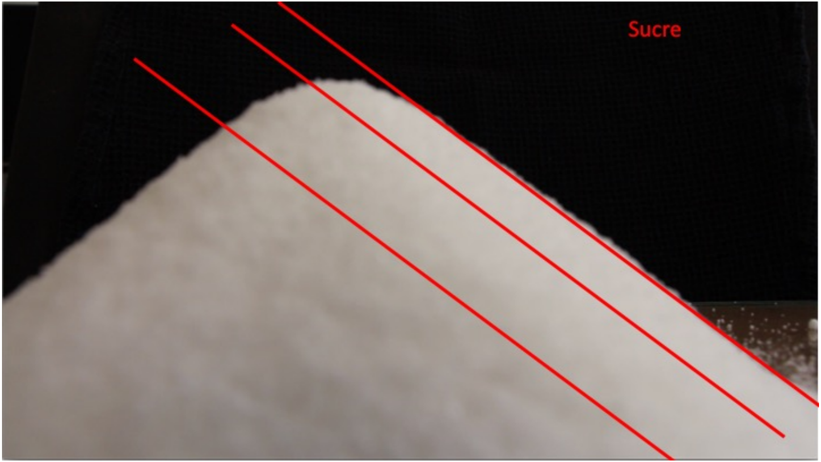
A complex behavior!



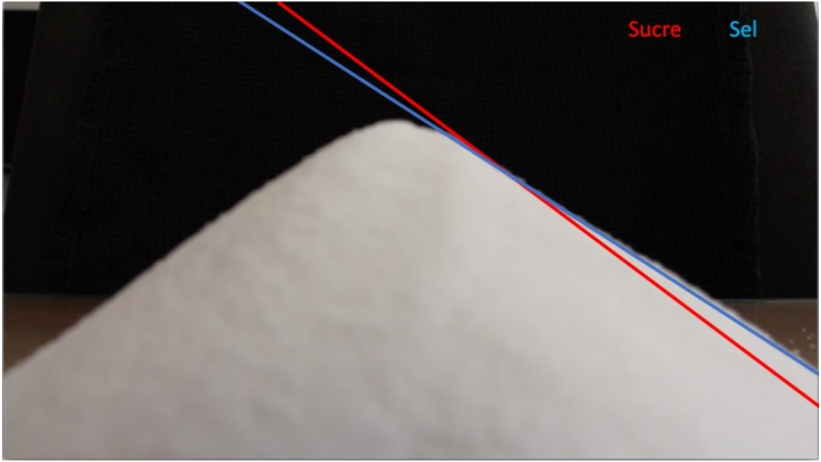
A complex behavior!



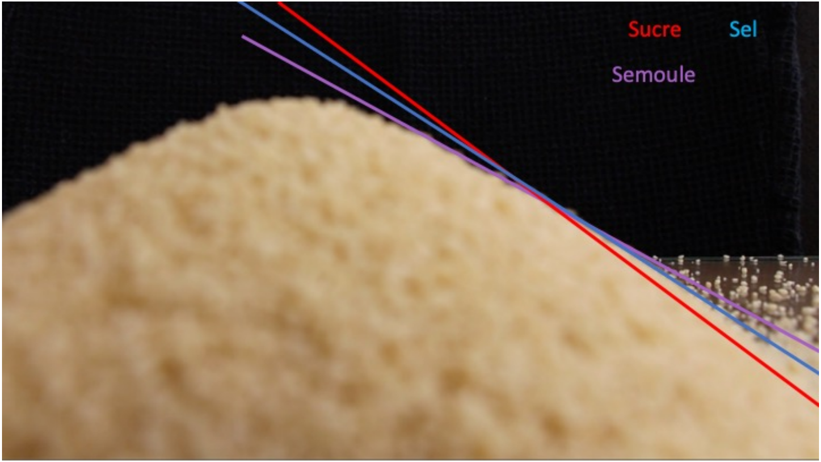
A complex behavior!



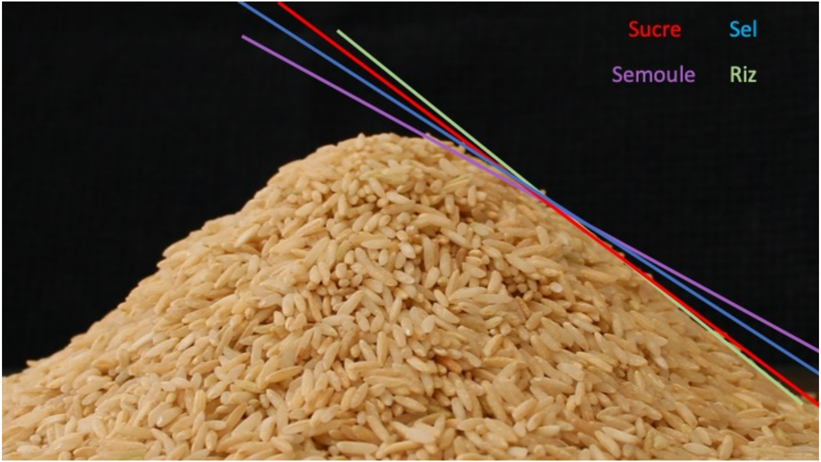
A complex behavior!



A complex behavior!

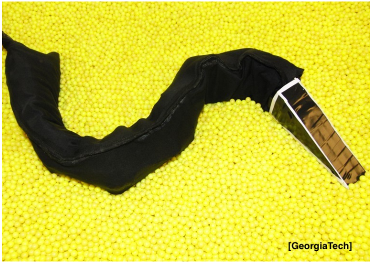


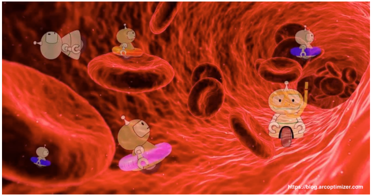
A complex behavior!



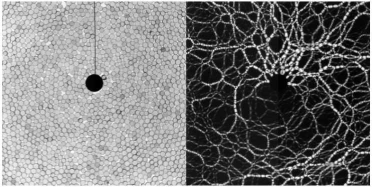
Liquid or solid?

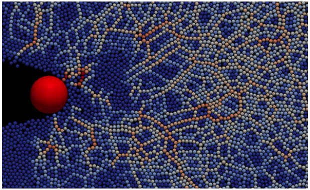
Learn to swim...





Using numerical simulations to understand...





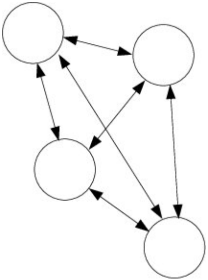
Why?

- Choice of physical models independently of experimental equipment
- Measurement error and noise
- Knowledge of all physical quantities

Difficulties:

- High number of particles
- Need for a detailed modelization of the physics
  Microscopic description
- Post-processing

$$m_i \frac{d\mathbf{x}_i}{dt} = F_i^{ext} + \sum_{i,j} F_{ij}^{contact}, \quad i = 1 \dots N$$



Particles in interaction.

Numerical complexity.

- High number of particles
- N^2 interactions
- Discontinuous forces

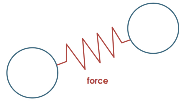
$\Longrightarrow$ Highly coupled / Non-linear

Two alternative classes of models

Molecular Dynamics (DEM)

[Cundall and Strack, 1979]

Contact = explicit force



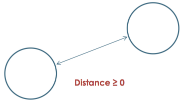
- Various models
  Easy to implement
- Continuous but very stiff
  Many parameters to choose

Contact Dynamics (NSCD)

[Moreau et Jean, 1992-1999]

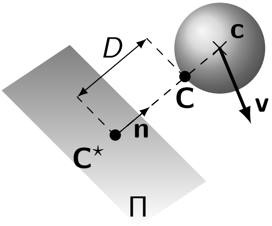
Constraint = positive distance

Contact = vanishing distance



- Stable, no parameter to tune
  Non-smooth convex analysis
- Only main features modeled
  Difficulty of implementation

Non Smooth Contact Dynamics for frictionless contacts



- **Contact force exerted on the particle:**

$$\mathbf{f} = f_n \, \mathbf{n} \quad \text{where} \quad f_n \in \mathbb{R}$$

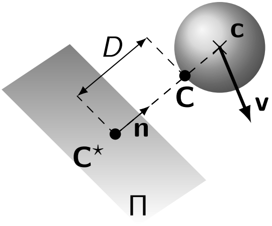
- **Admissible configurations:**

$$\mathcal{Q} = \left\{ \mathbf{c} \in \mathbb{R}^3, \quad D(\mathbf{c}) \geq 0 \right\}.$$

Signorini conditions

$$D(\mathbf{c}) \geq 0, \quad f_n \geq 0, \quad D(\mathbf{c}) \, f_n = 0$$

Inelastic contact law



- **Admissible velocities:**

$$\mathcal{C}_{\mathbf{c}} = \left\{ \mathbf{v} \in \mathbb{R}^3, \quad \nabla D(\mathbf{c}) \cdot \mathbf{v} \geq 0 \text{ if } D(\mathbf{c}) = 0 \right\}.$$

Contact law

$$\mathbf{v}^+ = P_{\mathcal{C}_{\mathbf{c}}} \mathbf{v}^-$$

- Relative velocity:

$$\nabla D(\mathbf{c}) \cdot \mathbf{v} \geq 0 \quad \Leftrightarrow \quad \mathbf{n} \cdot \mathbf{v} \geq 0 \quad \Leftrightarrow \quad \mathbf{n} \cdot \mathbf{v}_{\mathbf{C}} \geq 0$$

- Regularity issues...

The inelastic frictionless NSCD model

$$M\frac{d\mathbf{v}}{dt} = \mathbf{f}^{ext} + f_n\,\mathbf{n} \qquad \text{(FPD)}$$

$$D(\mathbf{c}) \geq 0, \quad f_n \geq 0, \quad D(\mathbf{c})\,f_n = 0 \qquad \text{(Singorini conditions)}$$

$$\mathbf{v}^+ = P_{\mathcal{C}_\mathbf{c}}\mathbf{v}^- \qquad \text{(Contact law)}$$

$$\text{where } \mathcal{C}_\mathbf{c} = \left\{\mathbf{v} \in \mathbb{R}^3, \quad \nabla D(\mathbf{c}) \cdot \mathbf{v} \geq 0 \text{ if } D(\mathbf{c}) = 0\right\}.$$

$\Longrightarrow$ Numerical scheme ?

Discretizing the constraint

- Admissible velocities

$$\mathcal{C}_{\mathbf{c}} = \left\{ \mathbf{v} \in \mathbb{R}^3, \quad \nabla D(\mathbf{c}) \cdot \mathbf{v} \geq 0 \text{ if } D(\mathbf{c}) = 0 \right\}.$$

Founding NSCD algorithms [Jean, Moreau, 1992, 1999]

$$K^k = \left\{ \mathbf{v} \in \mathbb{R}^3, \ \nabla D(\mathbf{c}^k) \cdot \mathbf{v} \geq 0 \text{ if } D(\mathbf{c}^k) \leq 0 \right\}$$

$\Longrightarrow$ Particles can overlap the plane.

Discretizing the constraint

- Admissible configurations

$$\mathcal{Q} = \left\{ \mathbf{c} \in \mathbb{R}^3, \quad D(\mathbf{c}) \geq 0 \right\}.$$

- $D(\mathbf{c}^{k+1}) = D(\mathbf{c}^k) + \triangle t \, \nabla D(\mathbf{c}^k) \cdot \mathbf{v} + O((\triangle t)^2) \geq 0,$

First order discretization [Maury, 2006]

$$K^k = \left\{ \mathbf{v} \in \mathbb{R}^3, \ D(\mathbf{c}^k) + \triangle t \, \nabla D(\mathbf{c}^k) \cdot \mathbf{v} \geq 0 \right\}.$$

$\Longrightarrow$ Feasible configurations.

A numerical scheme based on convex optimization

- Contact law: $\mathbf{v}^+ = P_{\mathcal{C}_\mathbf{c}} \mathbf{v}^-$

An implicit time stepping scheme [Maury, 2006]

$$\min_{\mathbf{v} \in K^k} J(\mathbf{v})$$

$$J(\mathbf{v}) = \frac{1}{2} \left\| \mathbf{v} - \mathbf{V}^{k+1} \right\|_M, \quad \mathbf{V}^{k+1} = \mathbf{v}^k + \triangle t \, M^{-1} \mathbf{f}^{ext},$$

$$K^k = \left\{ \mathbf{v} \in \mathbb{R}^3, \;\; D(\mathbf{c}^k) + \triangle t \, \nabla D(\mathbf{c}^k) \cdot \mathbf{v} \geq 0 \right\}.$$

Optimality conditions

Lagrange Multipliers

$$\min_{\mathbf{v}\in K} J(\mathbf{v})$$

$$K = \left\{\mathbf{v} \in \mathbb{R}^3,\ \ g(\mathbf{v}) \leq 0\right\}$$

where g is an affine function.

$\exists \lambda \in \mathbb{R}$ such that:

$$\begin{aligned} \nabla J(\mathbf{v}) &= -\lambda \nabla g(\mathbf{v}) \\ g(\mathbf{v}) &\leq 0, \quad \lambda \geq 0, \\ g(\mathbf{v})\,\lambda &= 0 \end{aligned}$$

$$J(\mathbf{v}) = \frac{1}{2}\left\|\mathbf{v} - \mathbf{V}^{k+1}\right\|_M$$

$$g(\mathbf{v}) = -D(\mathbf{c}^k) - \triangle t\, \nabla D(\mathbf{c}^k)\cdot \mathbf{v}$$

$$\begin{aligned} \nabla J(\mathbf{v}) &= M\mathbf{v} - M\mathbf{V}^{k+1} \\ &= M\mathbf{v} - M\mathbf{v}^k - \triangle t\, \mathbf{f}^{ext} \\ \nabla g(\mathbf{v}) &= -\triangle t\, \nabla D(\mathbf{c}^k) \\ &= -\triangle t\, \mathbf{n} \end{aligned}$$

$$M\mathbf{v} - M\mathbf{v}^k = \triangle t\, \mathbf{f}^{ext} + \triangle t\, \lambda \mathbf{n}$$

A discrete fundamental principle of dynamics

Model.

$$M\frac{d\mathbf{v}}{dt} = \mathbf{f}^{ext} + f_n\mathbf{n}$$

$$D(\mathbf{c}) \geq 0, \quad f_n \geq 0,$$

$$D(\mathbf{c})\, f_n = 0$$

$$\mathbf{v}^+ = P_{\mathcal{C}_\mathbf{c}}\mathbf{v}^-$$

Algorithm (Optimality condition).

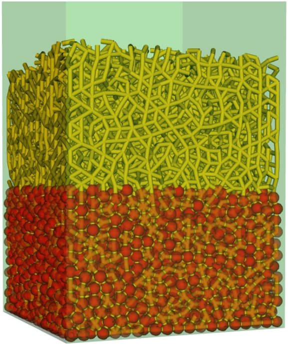
$$M\,\frac{\mathbf{v}^{k+1} - \mathbf{v}^k}{\triangle t} = \mathbf{f}^{ext} + f_n\mathbf{n}^k$$

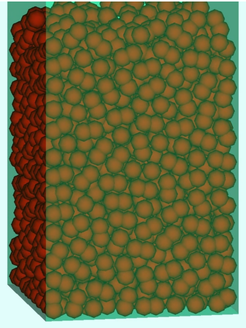
$$f_n \geq 0, \quad D(\mathbf{c}^k) + \triangle t\nabla D(\mathbf{c}^k)\cdot\mathbf{v}^{k+1} \geq 0,$$

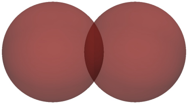
$$\left(D(\mathbf{c}^k) + \triangle t\nabla D(\mathbf{c}^k)\cdot\mathbf{v}^{k+1}\right) f_n = 0.$$

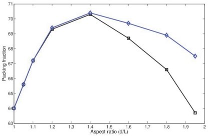
$\Longrightarrow$ Convergence results [Maury, 2006] [Bernicot, L, 2010]

Dynamic Numerical Investigation of Random Packing for Spherical and Nonconvex Particles



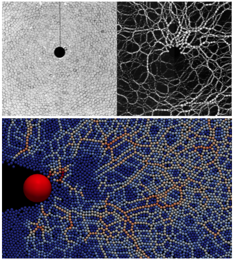


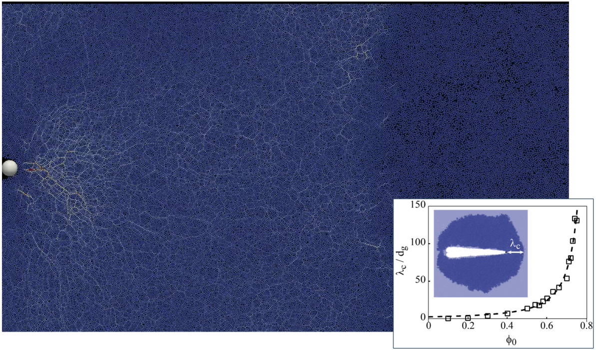




[S. Faure, A.L., B. Semin (2009)]   [SCoPI]

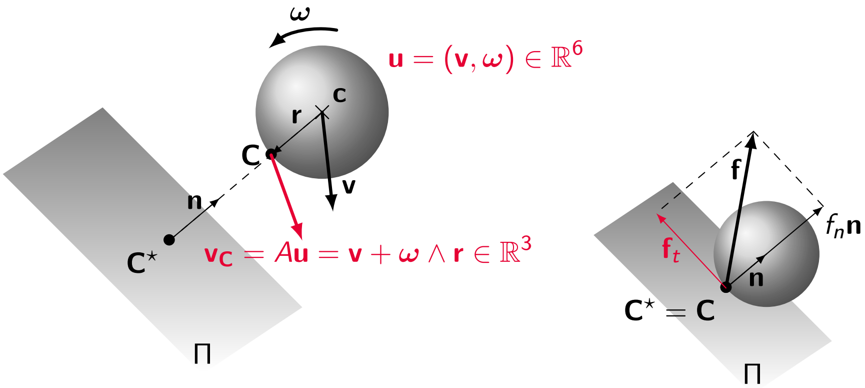
Clustering and flow around a sphere moving into a grain cloud





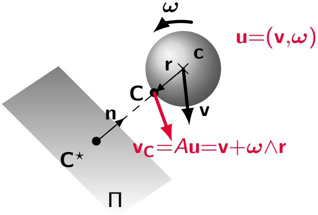
[A. Seguin, A.L., S. Faure, P. Gondret (2016)] [SCoPI]

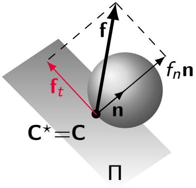
Modeling friction



[Hugo Martin (PhD), A.L., Yvon Maday, Anne Mangeney, Bertrand Maury]

Modeling friction





Normal contact law: inelastic collision.

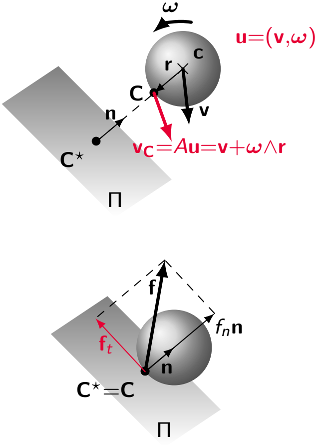
$$\mathbf{u}^+ = P_{\mathcal{C}_\mathbf{c}} \mathbf{u}^-$$

where

$$\mathcal{C}_\mathbf{c} = \{\mathbf{u} = (\mathbf{v}, \omega) \in \mathbb{R}^6, \\ \nabla_\mathbf{c} D(\mathbf{c}) \cdot \mathbf{v} \geq 0 \text{ if } D(\mathbf{c}) = 0\}.$$

$$[\mathbf{n} \cdot \mathbf{v_C} \geq 0]$$

Modeling friction



Tangential contact law: Coulomb law.

- If $P\mathbf{v_C}^+ \neq 0$ (sliding motion),

$$\mathbf{f}_t = -\mu f_n \frac{P\mathbf{v_C}^+}{|\,P\mathbf{v_C}^+\,|}$$

- If $P\mathbf{v_C}^+ = 0$ (no slip),

$$|\,\mathbf{f}_t\,| \leq \mu f_n$$

Modeling friction

$$M\frac{d\mathbf{u}}{dt} = \mathbf{F}^{ext} + A^T(f_n\mathbf{n} + \mathbf{f}_t) \qquad \text{(FPD)}$$

$$D(\mathbf{c}) \geq 0, \quad f_n \geq 0, \quad D(\mathbf{c})\, f_n = 0 \qquad \text{(Norm. cont.)}$$

$$\mathbf{u}^+ = P_{\mathcal{C}_\mathbf{c}}\mathbf{u}^-$$

$$\text{If} \quad PA\mathbf{u}^+ \neq 0 \text{ (sliding motion)}, \mathbf{f}_t = -\mu f_n \frac{PA\mathbf{u}^+}{|\, PA\mathbf{u}^+ \,|} \qquad \text{(Tang. cont)}$$

$$\text{If} \quad PA\mathbf{u}^+ = 0 \text{ (no slip)}\ , |\, \mathbf{f}_t \,| \leq \mu f_n$$

$$\left[\mathbf{u} = (\mathbf{v}, \omega), \quad A\mathbf{u} = \mathbf{v} + \omega \wedge \mathbf{r}, \quad A^T\mathbf{f} = (\mathbf{f}, \mathbf{r} \wedge \mathbf{f}) \in \mathbb{R}^6\right]$$

Founding NSCD algorithms [Jean, Moreau, 1992, 1999]

$$M \frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\triangle t} = \mathbf{F}^{ext} + A^{k,T}(f_n \mathbf{n}^k + \mathbf{f}_t) \qquad \text{(FPD)}$$

$$f_n \geq 0, \quad g(\mathbf{u}^{k+1}) \leq 0, \quad f_n\, g(\mathbf{u}^{k+1}) = 0 \qquad \text{(Norm. cont.)}$$

If $P^k A^k \mathbf{u}^{k+1} \neq 0$ (sliding motion), (Tang. cont)

$$\mathbf{f}_t = -\mu f_n \frac{P^k A^k \mathbf{u}^{k+1}}{|\, P^k A^k \mathbf{u}^{k+1} \,|}$$

If $P^k A^k \mathbf{u}^{k+1} = 0$ (no slip) , $|\, \mathbf{f}_t \,| \leq \mu f_n$

[Linear Complementarity Problem]

A convex formulation?

Lagrange Multipliers

$$\min_{\mathbf{u}\in K} J(\mathbf{u})$$

$$K = \{\mathbf{u} \in \mathbb{R}^6,\ \ g(\mathbf{u}) \leq 0\}$$

Under qualification conditions,

$\exists\lambda \in \mathbb{R}$ such that:

$$\nabla J(\mathbf{u}) = -\lambda \nabla g(\mathbf{u})$$
$$g(\mathbf{u}) \leq 0, \quad \lambda \geq 0,$$
$$g(\mathbf{u})\,\lambda = 0$$

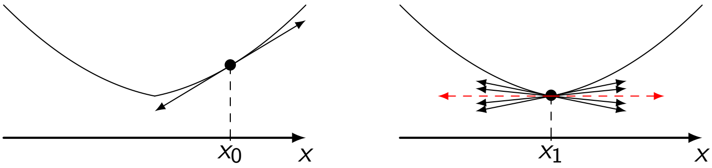
$$M\frac{d\mathbf{u}}{dt} = \mathbf{F}^{ext} + A^T(f_n\mathbf{n} + \mathbf{f}_t)$$

$$D(\mathbf{c}) \geq 0, f_n \geq 0, D(\mathbf{c})\,f_n = 0$$
$$\mathbf{u}^+ = P_{\mathcal{C}_\mathbf{c}}\mathbf{u}^-$$

$$PA\mathbf{u}^+ \neq 0,\ \ \mathbf{f}_t = -\mu f_n \frac{PA\mathbf{u}^+}{|\,PA\mathbf{u}^+\,|}$$
$$PA\mathbf{u}^+ = 0,\ \ |\,\mathbf{f}_t\,| \leq \mu f_n$$

$\Longrightarrow$ Need for non-derivable g.

Notion of subdifferential

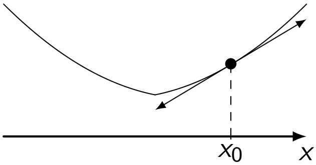


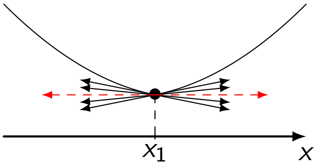
Sub-differential of a convex function

$\phi : \mathrm{R}^n \to \mathrm{R}$, convex function.

$$\partial\phi[\mathbf{x}] = \{\mathbf{y} \in \mathrm{R}^n / \quad \forall \hat{\mathbf{x}} \in \mathrm{R}^n, \quad \phi(\hat{\mathbf{x}}) \geq \phi(\mathbf{x}) + \mathbf{y} \cdot (\hat{\mathbf{x}} - \mathbf{x})\}$$

Notion of subdifferential





- **Example.** $\text{abs}(x) = |x|$

$$\partial\,\text{abs}[x] \underset{x>0}{=} \{1\}, \quad \partial\,\text{abs}[x] \underset{x<0}{=} \{-1\}, \quad \text{and} \quad \partial\,\text{abs}[0] = [-1, 1].$$

- **Optimality condition for a global minimization problem.**

$$\mathbf{x} \text{ is a minimum of } \phi \iff 0 \in \partial\phi[\mathbf{x}].$$

Optimality condition for non-derivable constraint

Lagrange Multipliers

$$\min_{\mathbf{u}\in K} J(\mathbf{u})$$

$$K = \left\{\mathbf{u} \in \mathbb{R}^6,\;\; g(\mathbf{u}) \leq 0\right\}$$

Under qualification conditions, $\exists \lambda \in \mathbb{R}$ such that:

$$\begin{aligned}
&\nabla J(\mathbf{u}) \in -\lambda\, \partial g[\mathbf{u}] \\
&g(\mathbf{u}) \leq 0, \quad \lambda \geq 0, \\
&g(\mathbf{u})\, \lambda = 0
\end{aligned}$$

$$\left.\begin{array}{l} \nabla J(\mathbf{u}) \in -\lambda\,\partial g[\mathbf{u}] \\ \lambda \geq 0, \quad g(\mathbf{u}) \leq 0 \\ \lambda\, g(\mathbf{u}) = 0 \end{array}\right\} \iff \begin{cases} M\dfrac{d\mathbf{u}}{dt} - \mathbf{F}^{ext} = A^T(f_n\mathbf{n} + \mathbf{f}_t) \\ f_n \geq 0,\ g(\mathbf{u}) \leq 0,\ f_n\, g(\mathbf{u}) = 0 \\ PA\mathbf{u}^+ \neq 0,\ \mathbf{f}_t = -\mu f_n \dfrac{PA\mathbf{u}^+}{|\,PA\mathbf{u}^+\,|} \\ PA\mathbf{u}^+ = 0,\ |\,\mathbf{f}_t\,| \leq \mu f_n \end{cases}$$

$$\begin{array}{l} \mathbf{f}_t = -\mu f_n \mathbf{w} \\ A^T(f_n\mathbf{n} + \mathbf{f}_t) = f_n\, A^T\,(\mathbf{n} - \mu\mathbf{w}) \end{array} \quad \left| \begin{array}{l} PA\mathbf{u}^+ \neq 0,\ \mathbf{w} = \dfrac{PA\mathbf{u}^+}{|\,PA\mathbf{u}^+\,|} \\ PA\mathbf{u}^+ = 0, \quad \mathbf{w} \in \Pi \text{ and } |\,\mathbf{w}\,| \leq 1 \end{array} \right.$$

$$\Longrightarrow \quad g(\mathbf{u}) = -D(\mathbf{c}^k) - \triangle t \nabla_{\mathbf{c}} D(\mathbf{c}^k) \cdot \mathbf{v} + \mu \triangle t |P^k A^k \mathbf{u}|$$

[Tassora, Negrut, Anitescu, 2008]

A convex minimization problem

Time-stepping scheme for frictional contact

$$\min_{\mathbf{u}\in K_\mu} J(\mathbf{u})$$

$$J(\mathbf{u}) = \frac{1}{2}\left\|\mathbf{u} - \mathbf{U}^{k+1}\right\|_M, \quad \mathbf{U}^{k+1} = \mathbf{u}^k + \triangle t M^{-1}\mathbf{F}^{ext},$$

$$K_\mu = \left\{\mathbf{u} = (\mathbf{v}, \boldsymbol{\omega}) \in \mathbb{R}^6,\;\; D(\mathbf{c}^k) + \triangle t \nabla_{\mathbf{c}} D(\mathbf{c}^k)\cdot \mathbf{v} \geq \mu \triangle t |P^k A^k \mathbf{u}|\right\}$$

Corresponding discrete FPD

$$M\,\frac{\mathbf{u}^{k+1}-\mathbf{u}^{k}}{\triangle t} = \mathbf{F}^{ext} + A^{k,T}(f_n\mathbf{n}^k + \mathbf{f}_t) \qquad \text{(FPD)}$$

$$f_n \geq 0, \quad f_n\, g(\mathbf{u}) = 0 \qquad \text{(Norm. cont.)}$$

$$D(\mathbf{c}^k) + \triangle t \nabla_{\mathbf{c}} D(\mathbf{c}^k)\cdot \mathbf{v}^{k+1} \geq \mu \triangle t |P^k A^k \mathbf{u}^{k+1}|$$

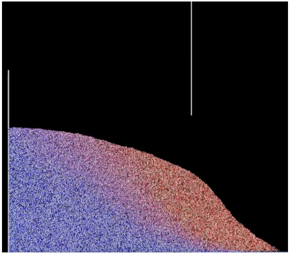
If $P^k A^k \mathbf{u}^{k+1} \neq 0$ (sliding motion), (Tang. cont)

$$\mathbf{f}_t = -\mu f_n \frac{P^k A^k \mathbf{u}^{k+1}}{|\,P^k A^k \mathbf{u}^{k+1}\,|}$$

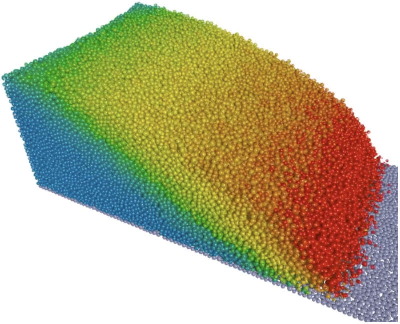
If $P^k A^k \mathbf{u}^{k+1} = 0$ (no slip) $,|\,\mathbf{f}_t\,| \leq \mu f_n$

Application to collapse and erodible beds

- Spherical particles
- 2D and 3D simulations
- Mosek solver



2D simulation - 70 000 spheres.



3D simulation - 112 000 spheres.

[**Hugo Martin** (PhD, LJLL, IPGP)]

On-going work and prospects

- Multiparticle case: links between the different discrete formulations.
  [with B. Maury]
- Extension to non-spherical particles (super-ellipsoids)
  [with S. Faure and L. Gouarin]
- Coupling with a fluid solver (CAFES, [L. Gouarin])