



Contacts: Numerical schemes based on convex optimization problems

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CMAP – Ecole Polytechnique

CEMRACS 2022

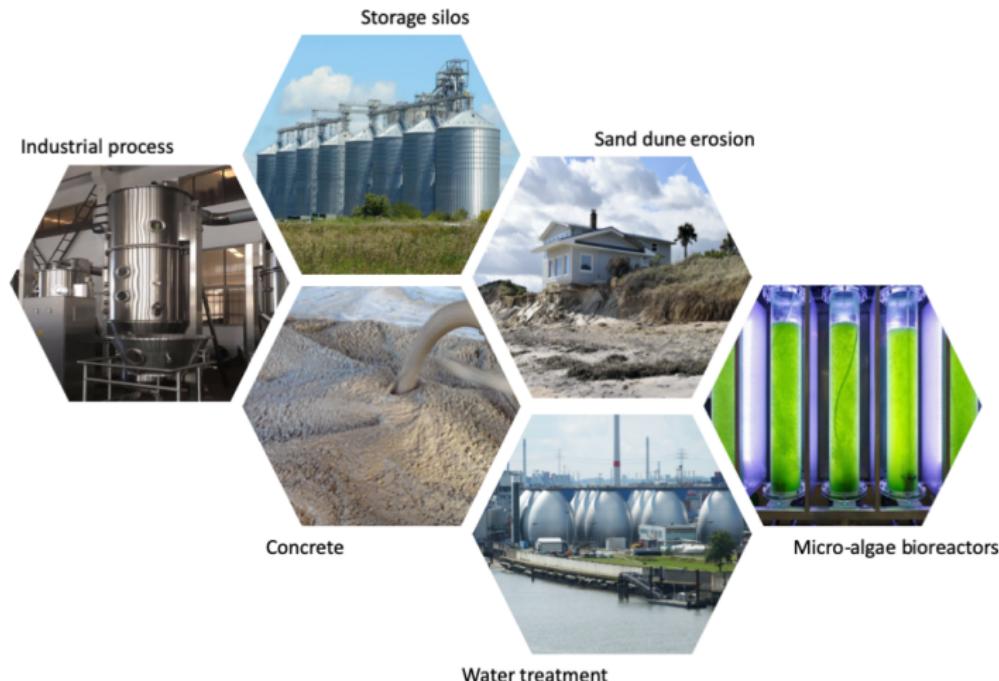
July 26, 2022

Joint work with: Hélène Bloch (CMAP) - Sylvain Faure (LMO, Orsay) - Philippe Gondret (FAST, Orsay) - Loïc Gouarin (CMAP) - Hugo Martin (IPGP) - Bertrand Maury (LMO, Orsay) - Antoine Seguin (FAST, Orsay) - Benoît Semin (PMMH, ESPCI)



ANR
RheoSuNN

Why study granular media?



Rheology

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

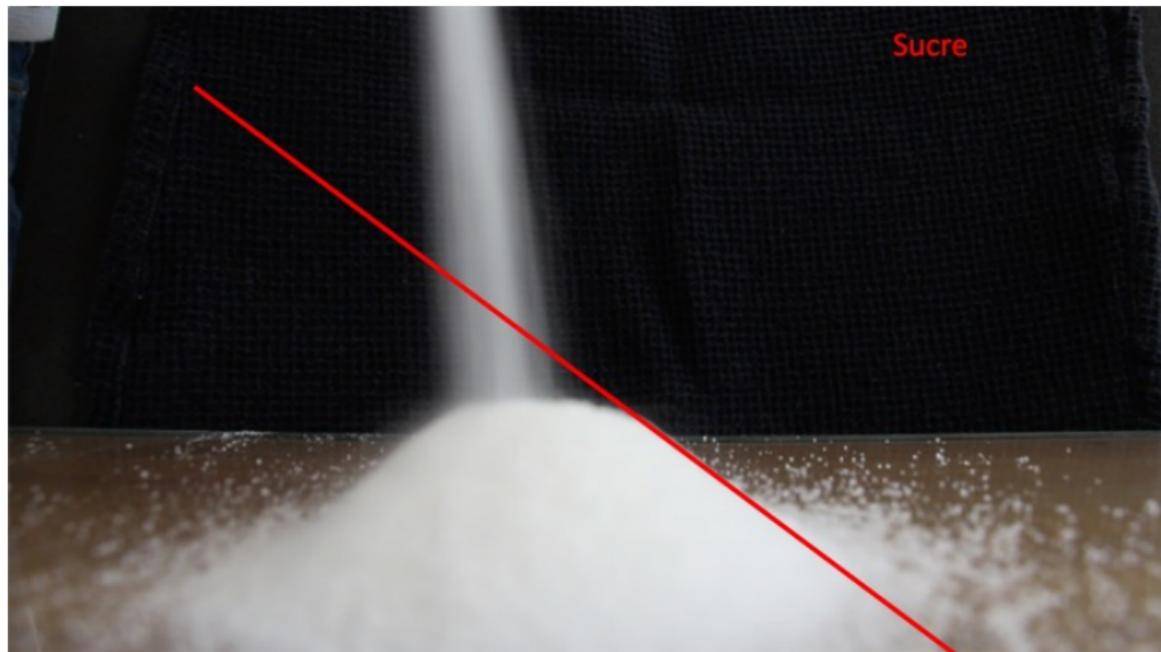
- ▶ flow, segregation, mixing, blocking, collapse...

Macroscopic behaviour

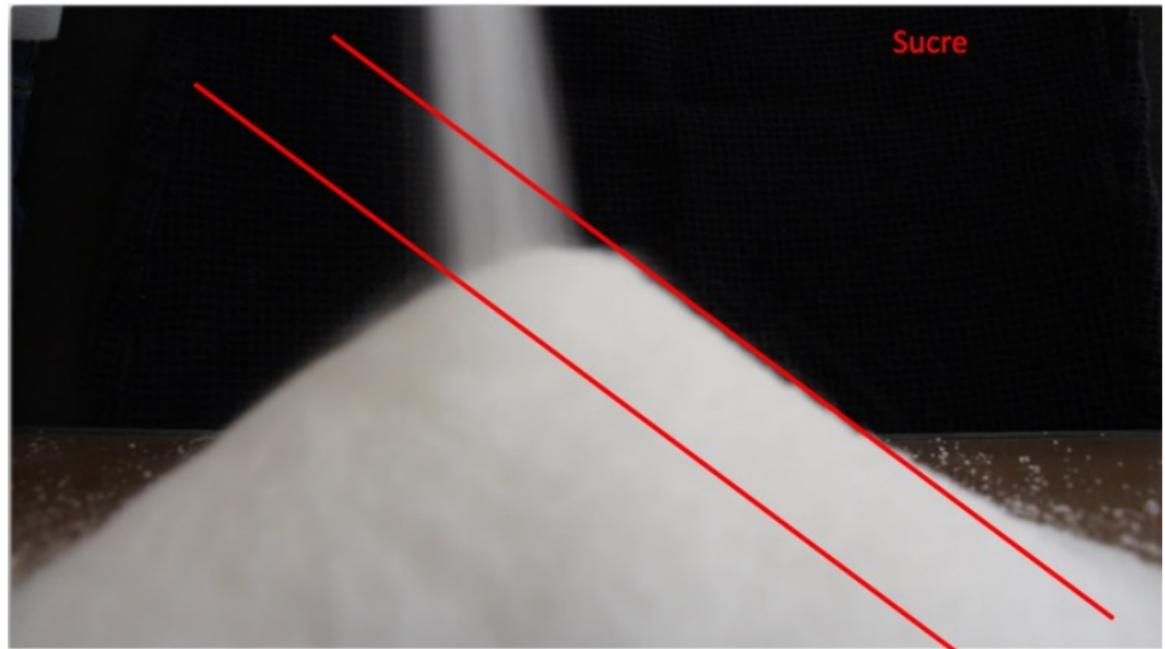
⇒ Still not well understood

⇒ Active domain of research

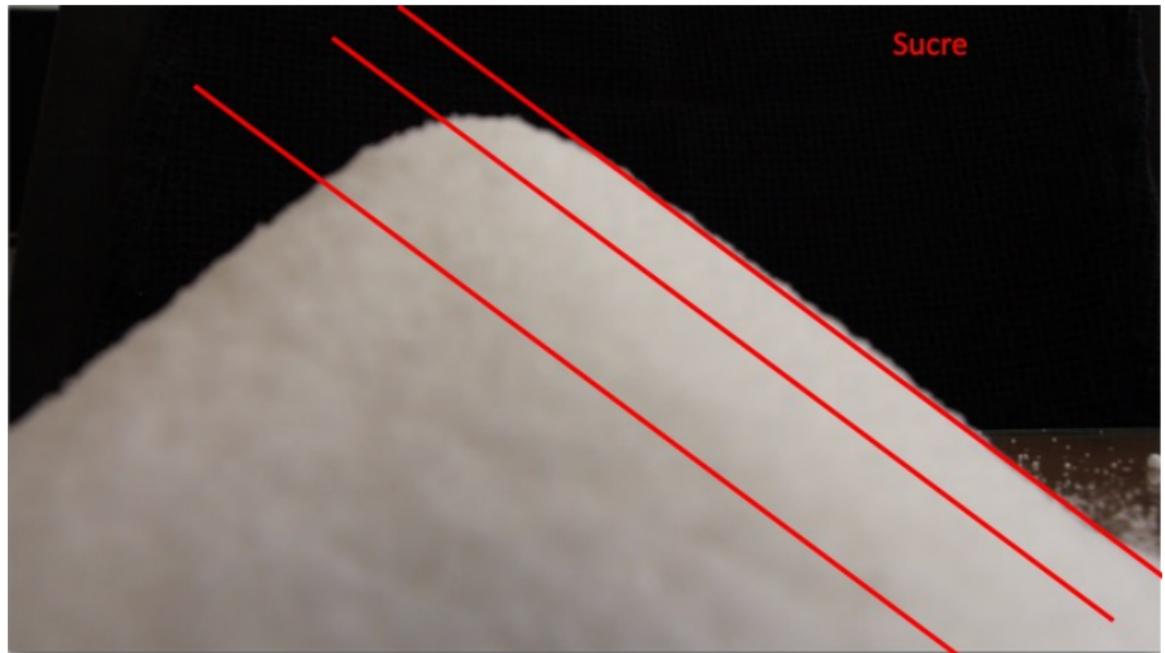
A complex behavior!



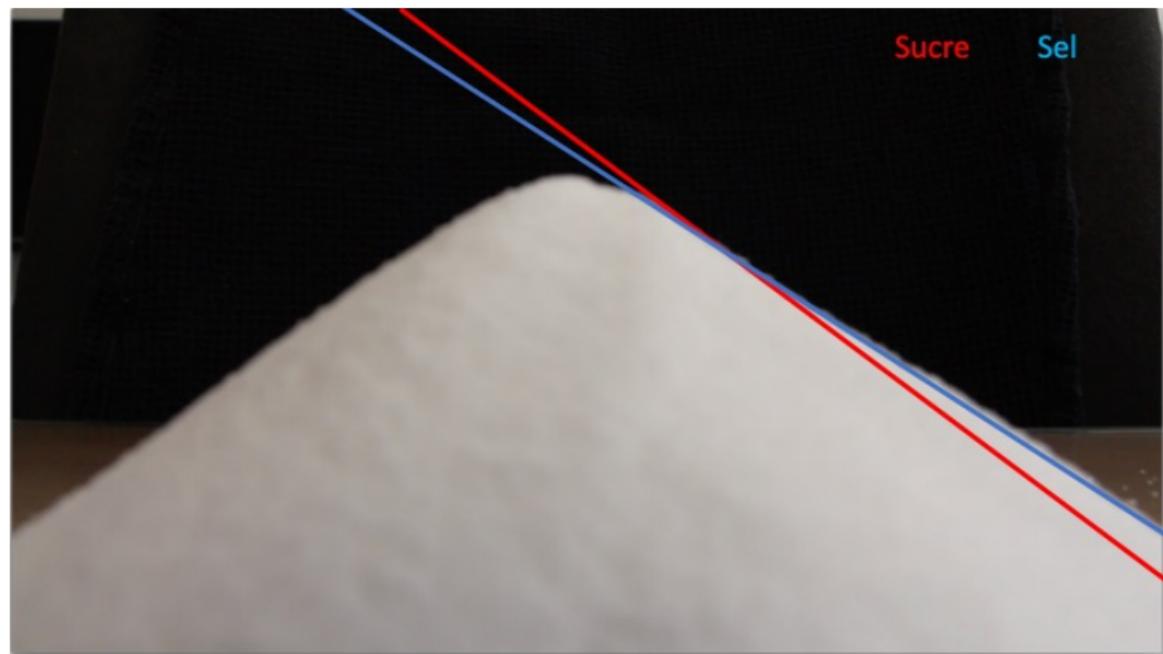
A complex behavior!



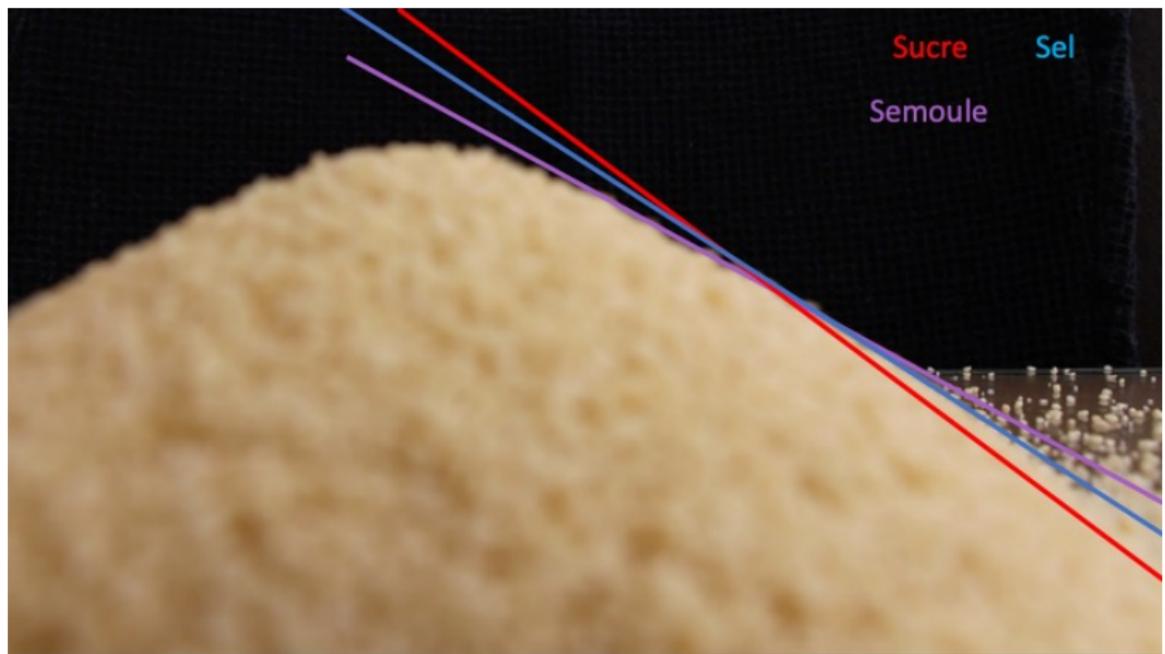
A complex behavior!



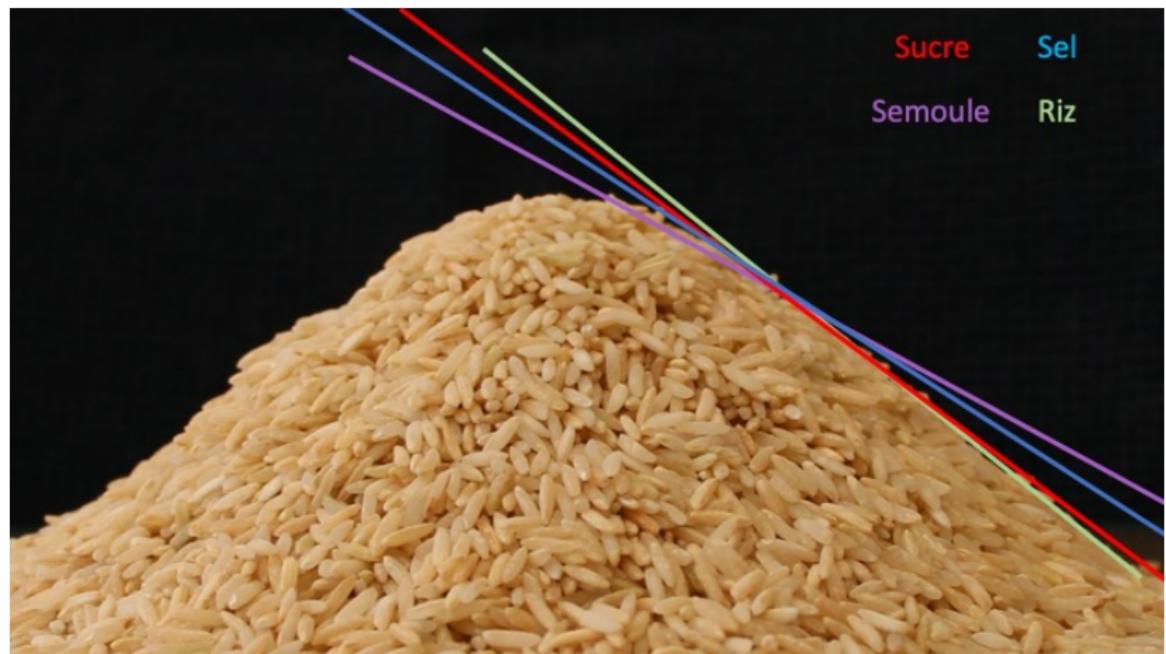
A complex behavior!



A complex behavior!



A complex behavior!



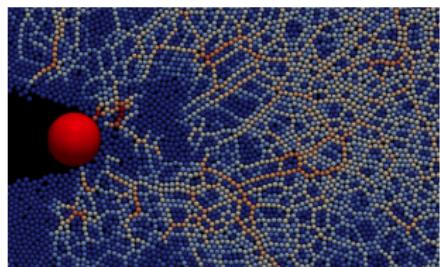
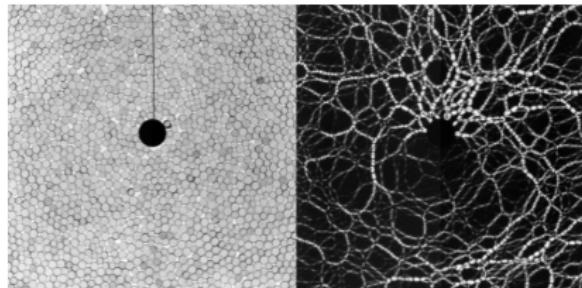
Liquid or solid?



Learn to swim...



Using numerical simulations to understand...



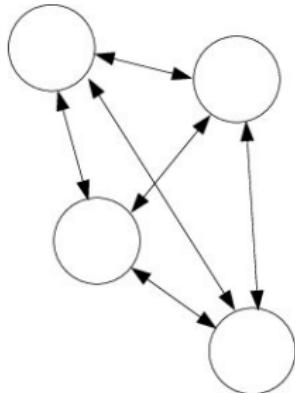
Why?

- Choice of physical models independently of experimental equipment
- No 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

$$m_i \frac{d^2 \mathbf{x}_i}{dt^2} = F_i^{\text{ext}} + \sum_{i,j} F_{ij}^{\text{contact}}, \quad i = 1 \dots N$$



Particles in interaction.

Numerical complexity.

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

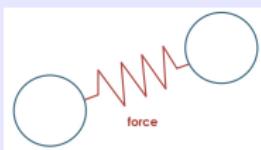
⇒ Highly coupled / Non-linear

Two alternative classes of models

Molecular Dynamics (MD)

[Cundall and Strack, 1979]

Contact = explicit force

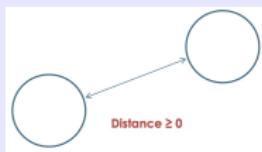


- ▶ Various models
Easy to implement
- ▶ Continuous but very stiff
Many parameters to choose

Contact Dynamics (NSCD)

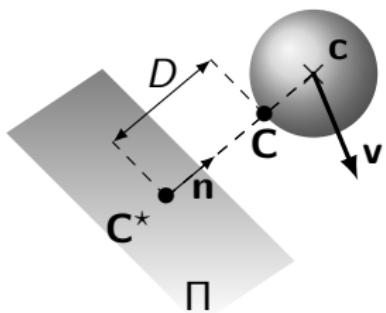
[Moreau et Jean, 1992-1999]

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:**

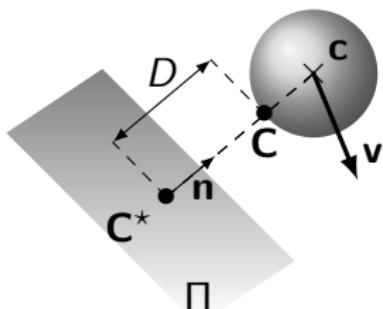
$$\mathcal{Q} = \{\mathbf{c} \in \mathbb{R}^3, \quad D(\mathbf{c}) \geq 0\}.$$

Signorini conditions

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

Looks like Lagrange multiplier and complementarity condition...

Inelastic contact law



► **Admissible velocities:**

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

Contact law

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

- $\nabla D(\mathbf{c}) \cdot \mathbf{v}^- < 0 \Rightarrow \nabla D(\mathbf{c}) \cdot \mathbf{v}^+ = 0 \Rightarrow \mathbf{n} \cdot \mathbf{v}^+ = 0$
- Regularity issues...

The inelastic frictionless NSCD model

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

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

$$\mathbf{v}^+ = P_{\mathcal{C}_c} \mathbf{v}^- \quad (\text{Contact law})$$

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

⇒ 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]

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

⇒ Particles can overlap the plane.

Discretizing the constraint

- ▶ Admissible configurations

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

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

First order discretization [Maury, 2006]

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

⇒ Feasible configurations.

A numerical scheme based on convex optimization

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

An implicit time stepping scheme [Maury, 2006]

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

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

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

Optimality conditions

Lagrange Multipliers

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

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

where g is an affine function.

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

$$\nabla J(\mathbf{v}) = -\lambda \nabla g(\mathbf{v})$$

$$g(\mathbf{v}) \leq 0, \quad \lambda \geq 0,$$

$$g(\mathbf{v}) \lambda = 0$$

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

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

$$\nabla J(\mathbf{v}) = M\mathbf{v} - M\mathbf{V}^{k+1}$$

$$= M\mathbf{v} - M\mathbf{v}^k - \Delta t \mathbf{f}^{ext}$$

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

$$= -\Delta t \mathbf{n}$$

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

A discrete fundamental principle of dynamics

Model.

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

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

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

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

Algorithm (Optimality condition).

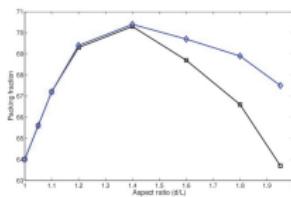
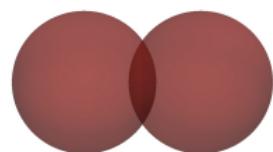
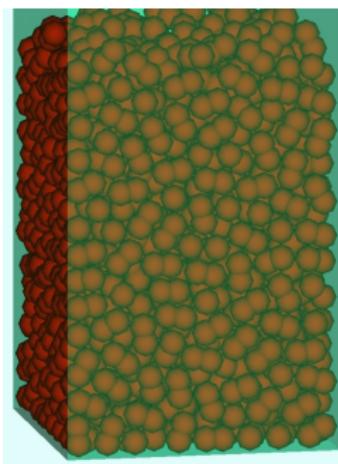
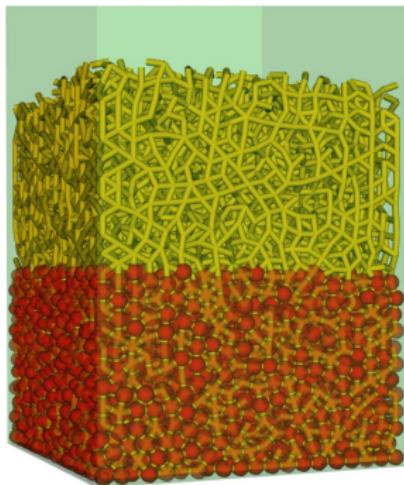
$$M \frac{\mathbf{v}^{k+1} - \mathbf{v}^k}{\Delta t} = \mathbf{f}^{ext} + f_n \mathbf{n}^k$$

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

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

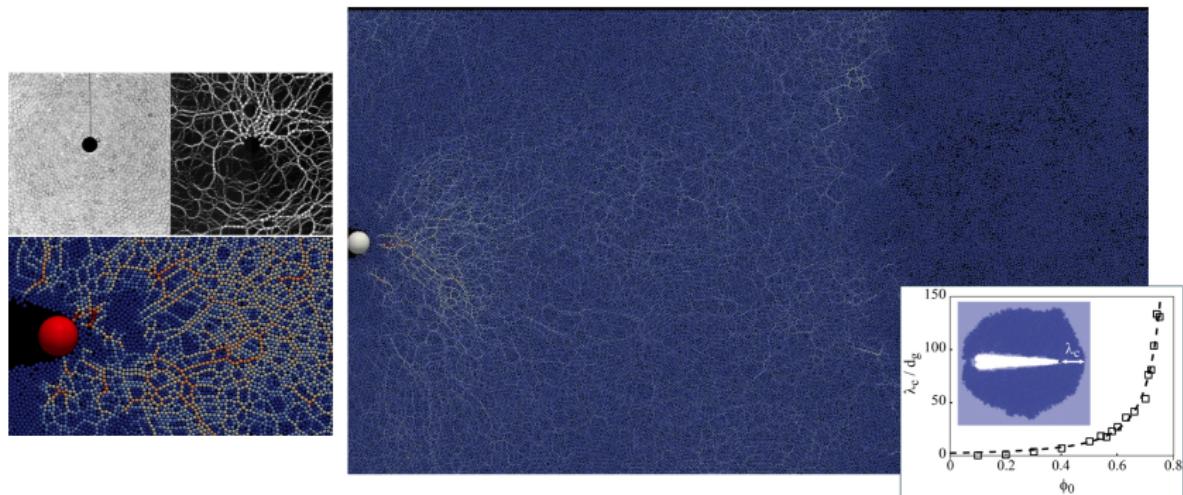
⇒ Convergence results [Maury, 2006] [Bernicot, L, 2010]

Dynamic Numerical Investigation of Random Packing for Spherical and Nonconvex Particles



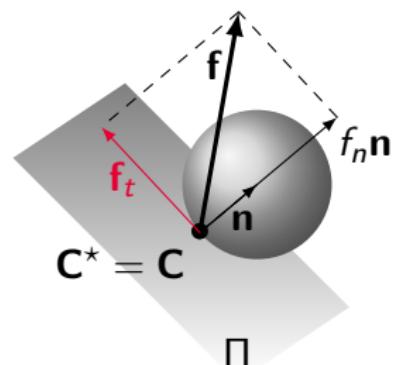
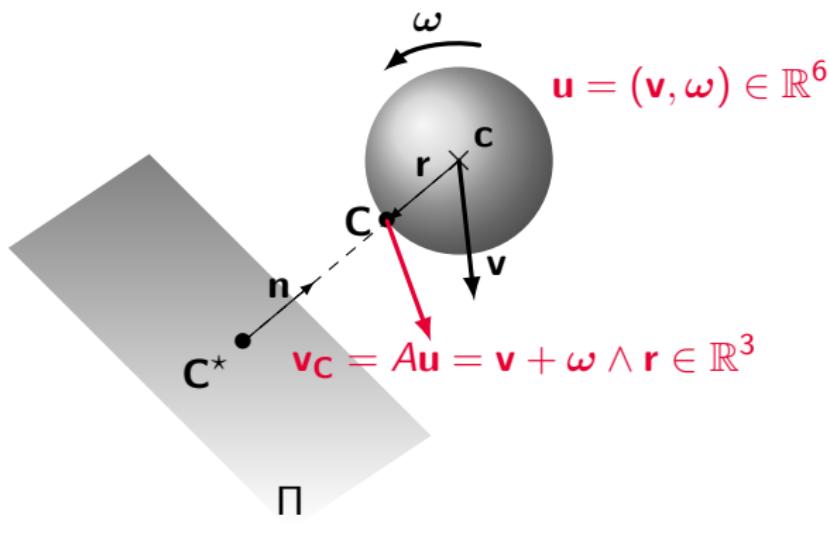
[S. Faure, A.L., B. Semin (2009)] [SCoPI]

Clustering and flow around a sphere moving into a grain cloud



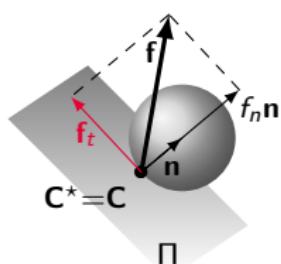
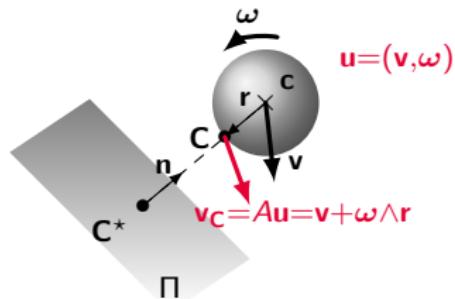
[A. Seguin, A.L., S. Faure, P. Gondret (2016)] [SCoPI]

Modeling friction



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

Modeling friction



Normal contact law: inelastic collision.

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

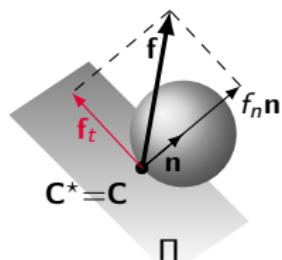
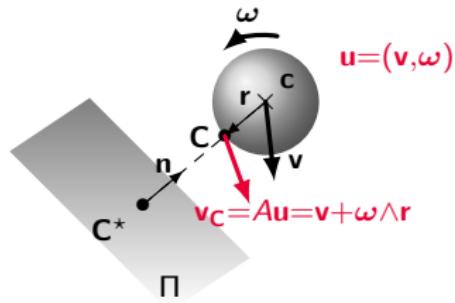
where

$$\mathcal{C}_c = \{\mathbf{u} = (\mathbf{v}, \omega) \in \mathbb{R}^6,$$

$$\nabla_{\mathbf{c}} D(\mathbf{c}) \cdot \mathbf{v} \geq 0 \text{ if } D(\mathbf{c}) = 0\}.$$

$$[\mathbf{n} \cdot \mathbf{v}_C \geq 0]$$

Modeling friction



Tangential contact law: Coulomb law.

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

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

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

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

Modeling friction

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

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

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

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

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

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

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

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

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

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:

$$\nabla J(\mathbf{u}) = -\lambda \nabla g(\mathbf{u})$$

$$g(\mathbf{u}) \leq 0, \quad \lambda \geq 0,$$

$$g(\mathbf{u}) \lambda = 0$$

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

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

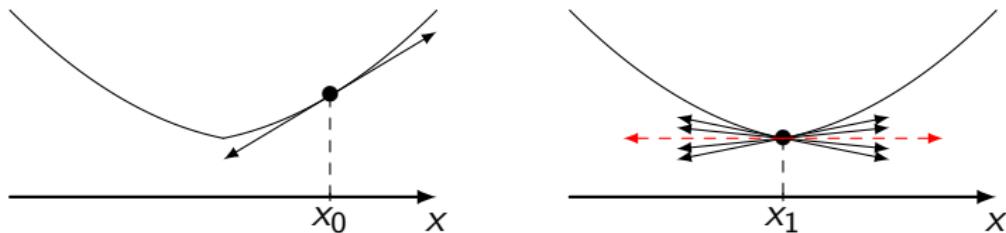
$$\mathbf{u}^+ = P_{\mathcal{C}_c} \mathbf{u}^-$$

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

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

\implies Need for non-derivable g .

Notion of subdifferential

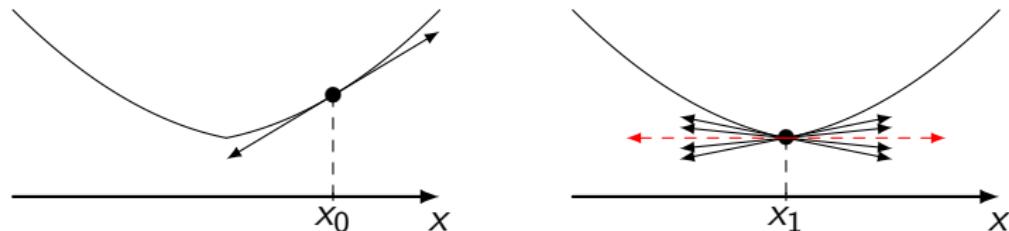


Sub-differential of a convex function

$\phi : \mathbb{R}^n \rightarrow \mathbb{R}$, convex function.

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

Notion of subdifferential



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

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

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

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

Optimality condition for non-derivable constraint

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:

$$\nabla J(\mathbf{u}) \in -\lambda \partial g[\mathbf{u}]$$

$$g(\mathbf{u}) \leq 0, \quad \lambda \geq 0,$$

$$g(\mathbf{u}) \lambda = 0$$

$$\left. \begin{array}{l} \nabla J(\mathbf{u}) \in -\lambda \partial g[\mathbf{u}] \\ \lambda \geq 0, \quad g(\mathbf{u}) \leq 0 \\ \lambda g(\mathbf{u}) = 0 \end{array} \right\} \iff \left\{ \begin{array}{l} M \frac{d\mathbf{u}}{dt} - \mathbf{F}^{ext} = A^T (f_n \mathbf{n} + \mathbf{f}_t) \\ f_n \geq 0, \quad g(\mathbf{u}) \leq 0, \quad f_n g(\mathbf{u}) = 0 \\ PA\mathbf{u}^+ \neq 0, \quad \mathbf{f}_t = -\mu f_n \frac{PA\mathbf{u}^+}{|PA\mathbf{u}^+|} \\ PA\mathbf{u}^+ = 0, \quad |\mathbf{f}_t| \leq \mu f_n \\ PA\mathbf{u}^+ \neq 0, \quad \mathbf{w} = \frac{PA\mathbf{u}^+}{|PA\mathbf{u}^+|} \\ PA\mathbf{u}^+ = 0, \quad \mathbf{w} \in \Pi \text{ and } |\mathbf{w}| \leq 1 \end{array} \right.$$

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

[Tassora, Negrut, Anitescu, 2008]

A convex minimization problem

Time-stepping scheme for frictional contact

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

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

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

Corresponding discrete FPD

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

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

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

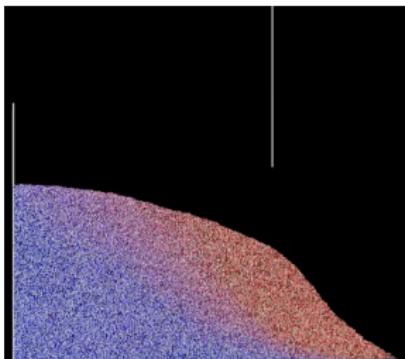
If $P^k A^k \mathbf{u}^{k+1} \neq 0$ (sliding motion), (Tang. cont)

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

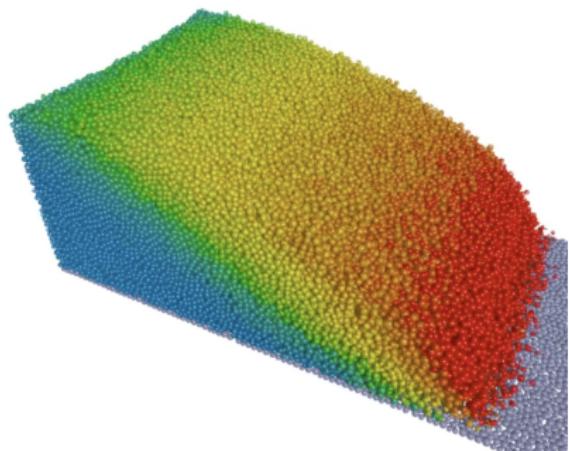
If $P^k A^k \mathbf{u}^{k+1} = 0$ (no slip), $|\mathbf{f}_t| \leq \mu f_n$

Application to collapse and erodible beds

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



2D simulation - 70 000 spheres.

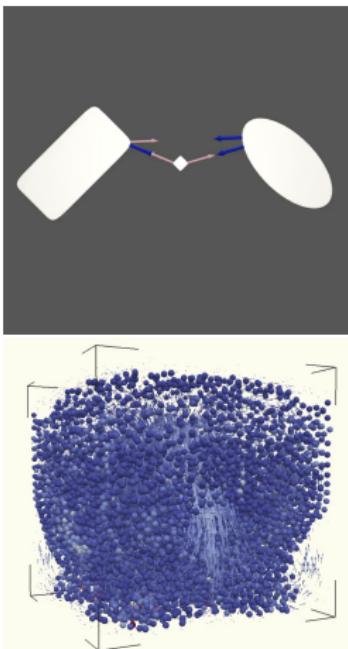


3D simulation - 112 000 spheres.

[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, L. Gouarin, H. Bloch]
- ▶ Coupling with viscous contact model
[with H. Bloch]
- ▶ Coupling with a fluid solver
(CAFES, [L. Gouarin, H. Bloch])



CEMRACS Project

Modelling, analysis, and simulation of traffic jam in colonies of *Myxococcus xanthus*

- ▶ Rippling phase: bacteria synchronize in accordion waves
- ▶ Repeated reversions of individual bacteria
- ▶ Model for reversions? Due to contacts?

Project proposed by: A. L.-L., Vincent Calvez

Team: Hélène Bloch, Benoît Gaudeul, Michèle Romanos, Jean-Baptiste Saulnier

