Direct numerical simulation of granular media and suspensions

Taking close interactions into account

Ecole 2022 du GdR MathGeoPhy

Aline Lefebvre - Lepot
28 octobre 2022
Suspensions and granular media.

Macroscopic, non-brownian entities
Rheology: ”the branch of physics concerned with the flow and change of shape of matter”

[Collins English Dictionary]

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

**Macroscopic behaviour**
A complex behaviour!


Multi-particle interactions
Contact Friction
Shape of particles
Local micro-structure
Non-local effects

Active domain of research
Need for numerical simulations
Numerical simulations. The difficulties.

- Macroscopic behaviour
- Steady state and time average

⇒ Large number of particles
⇒ Long time simulations

Need for fast N-body computations
Numerical simulations. The difficulties.

- Dense suspensions → Close interactions due to the fluid

Need for methods taking lubrication into account
Numerical simulations. The difficulties.

- Dense suspensions
- Granular media

⇒ Solid contacts between particles

Molecular Dynamics

Explicit force

Continuous penalization method

[Cundall, Strack, 1979]

Contact law

Inelastic contacts
Coulomb friction law

Explicit solution for 2 particles

Multi-contact problem

Need for a stable algorithm to deal with contacts
Overview.

Granular media
- Rheological study
  - S. Faure, P. Gondret, A. Seguin
- Granular collapse
  - PhD H. Martin, Y. Maday, A. Mangeney, B. Maury

Suspensions
- Solid contacts
- Lubrication
- Direct fluid solvers
- RheoSuNN
- Anti-rheology
- Inelastic contact
  - [B. Maury]
- Frictional contact
  - PhD H. Martin, Y. Maday, A. Mangeney, B. Maury
- Gluey contact
  - [B. Maury]
- Lubrication effects on the flow
  - [B. Merlet, F. Nabet, F. Vergnet]
- BEM solvers
  - [F. Alouges, M. Aussal, F. Pigeonneau, A. Sellier, L. Faria]
- FEM solvers
  - CAFES
  - [B. Fabrèges, L. Gouarin]

SCoPI

ANR RheoSuNN
Taking lubrication into account in the fluid solver.

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- **A singular problem**
  - Correction of the flow?
  - Non-spherical particles?

\[ -\mu \Delta \mathbf{u} + \nabla p = 0 \quad \text{in } \mathcal{F} \]
\[ \nabla \cdot \mathbf{u} = 0 \quad \text{in } \mathcal{F} \]
\[ \mathbf{u} = \mathbf{u}^* \quad \text{on } \partial B \]

\[ \| \mathbf{u} - \mathbf{u}_h \| \leq C \| (\mathbf{u}, p) \| h^\alpha \]

Blows up when the distance goes to zero…

**An accurate method to include lubrication forces in numerical simulations of dense suspensions.** With B. Merlet, and T. N. Nguyen. JFM, 769 (2015)
Taking lubrication into account in the fluid solver.

\[
(u_h^{\text{new}}, p_h^{\text{new}}) = (u^{\text{sing}}, p^{\text{sing}}) + (u_h^{\text{reg}}, p_h^{\text{reg}})
\]

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\[(u_{h}^{\text{new}}, p_{h}^{\text{new}}) = (u^{\text{sing}}, p^{\text{sing}}) + (u_{h}^{\text{reg}}, p_{h}^{\text{reg}})\]

\[-\mu \Delta u^{\text{reg}} + \nabla p^{\text{reg}} = \mu \Delta u^{\text{sing}} - \nabla p^{\text{sing}} \quad \text{in } \mathcal{F}\]

\[\nabla \cdot u^{\text{reg}} = -\nabla \cdot u^{\text{sing}} \quad \text{in } \mathcal{F}\]

\[u^{\text{reg}} = u^{*} - u^{\text{sing}} \quad \text{on } \partial B\]
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\[\nabla \cdot u^{\text{reg}} = -\nabla \cdot u^{\text{sing}} \quad \text{in } \Omega\]
\[u^{\text{reg}} = u^{\ast} - u^{\text{sing}} \quad \text{on } \partial B\]

\[\|u - u_{h}^{\text{new}}\| \leq C \|(u^{\text{reg}}, p^{\text{reg}})\| h^{\alpha}\]

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Stable and convex contact algorithms.

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ANR RheoSuNN

Inelastic contact

Frictional contact

Granular collapse
Stable and convex contact algorithms.

Multi-contact problem

Inelastic contacts
Coulomb law

Non-Smooth Contact Dynamics

Implicit force
\[ d \geq 0 \]

Non-smooth convex analysis
[Moreau, Jean, 1992-1999]
Stable and convex contact algorithms.

Inelastic contact

\[
\min_{v \in K} \frac{1}{2} \| v - v^{k+1} \|_M
\]

\[
K = \{ v, \quad D^k + dt \nabla D^k \cdot v \geq 0 \}
\]

Inelastic contact with friction


An optimization-based model for dry granular flows: application to granular collapse on erodible beds, with H. Martin, A. Mangeney, Y. Maday, B. Maury, Submitted.
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Inelastic contact

\[
\min_{v \in K} \frac{1}{2} \|v - V^{k+1}\|_M
\]

\[
K = \{v, \ D^k + dt \nabla D^k \cdot v \geq 0\}
\]

Inelastic contact with friction

Linear constraint

SCoPI


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Inelastic contact

\[ \min_{v \in K} \frac{1}{2} \| v - v^{k+1} \|_M \]

\[ K = \{ v, \ D^k + dt \nabla D^k \cdot v \geq 0 \} \]

Inelastic contact with friction

\[ \min_{v \in K_\mu} \frac{1}{2} \| u - U^{k+1} \|_M \]

\[ K_\mu = \{ u, \ D^k + dt \nabla D^k \cdot v \geq \mu dt |Tu| \} \]

SCoPI

[H. Martin]

\[ \frac{v^{k+1} - v^k}{dt} = f_{ext} + f_n n^k \]

\[ D^k + dt \nabla D^k \cdot v^{k+1} \geq 0 \]

\[ f_n \geq 0 + \text{compl.} \]

[Maury, 2006]


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**Inelastic contact**

\[
\min_{v \in K} \frac{1}{2} \| v - v^{k+1} \|_M
\]

\[K = \{ v, \; D^k + dt \nabla D^k \cdot v \geq 0 \}\]

- Implicit algorithms
- No need to detect the contacts times
- Convex minimization problems at each time step

\[
m \frac{v^{k+1} - v^k}{dt} = f_{ext} + f_n n^k
\]

\[D^k + dt \nabla D^k \cdot v^{k+1} \geq 0\]

\[f_n \geq 0 + \text{compl.}\]

[Maury, 2006]

**Inelastic contact with friction**

\[
\min_{v \in K_\mu} \frac{1}{2} \| u - U^{k+1} \|_M
\]

\[K_\mu = \{ u, \; D^k + dt \nabla D^k \cdot v \geq \mu dt |T u| \}\]

- Linear constraint
- Conic constraint

**SCoPi**

[H. Martin]

- Implicit algorithms
- No need to detect the contacts times
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\[
m \frac{v^{k+1} - v^k}{dt} = f_{ext} + (f_n n^k + f_t)
\]

\[J \frac{\omega^{k+1} - \omega^k}{dt} = r \wedge (f_n n^k + f_t)\]

\[D^k + dt \nabla D^k \cdot v^{k+1} \geq \mu dt |T u^{k+1}|\]

\[f_n \geq 0 + \text{compl.}\]

**Coulomb** \((v^{k+1}, \omega^{k+1}, f_n, f_t)\)

[Tassora, Negrut, Anitescu, 2008]
Stable and convex contact algorithms.

- Inelastic contacts
- Spherical particles
- SCoPI

Rheology

Chains of forces

Clustering and flow around a sphere moving into a grain cloud. With A. Seguin, S. Faure, and P. Gondret.
In: The European Physical Journal E 39.6 (2016)
Stable and convex contact algorithms.

Friction  Spherical particles  Hugo Martin [LJLL, IPGP]

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- Convergence
- Non-spherical particles
- Hélène Bloch [CMAP]

\[ D^k + d t \nabla D^k \cdot v^{k+1} \geq \mu d t |Tu^{k+1}| \]

- Influence of convexification?
- Very few convergence results based on compacity methods
- Order of convergence?

Numerical study:
\[ \text{err} = O(dt) \]

On convex numerical schemes for inelastic contacts with friction, with H. Bloch, Proceeding SMAI2021, Submitted
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Coupling with the gluey particle model

Numerical simulation of gluey particles, M2AN 43 (2009)
Stable and convex contact algorithms.

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Numerical simulation of gluey particles, M2AN 43 (2009)
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耦合与粘性粒子模型
**Stable and convex contact contact algorithms.**

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- Coupling gluey and frictional contacts
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**Suspensions**
- **Lubrication**
  - Lubrication effects on the flow
    - [B. Merlet, F. Nabet, F. Vergnet]
  - Extension to fictitious domain solvers
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