Contact Dynamics and Plastic Granular Flows

Farhang Radjaï
University of Montpellier - CNRS, LMGC, France

Stéphane Roux
LMT-Cachan, CNRS, ENS de Cachan, France

Vincent Richefeu (3SR, Grenoble), Emilien Azéma (LMGC, Montpellier), Jean-Yves Delenne (INRA, Montpellier), Nicolas Berger (LMGC, Montpellier)
Introduction

Does a collection of infinitely rigid particles represent a physically valid picture of granular materials?

Plastic behavior with no elastic domain

DEM simulation with no force law

Elastic deflections can be made as small as possible: \[ \frac{p}{E} \rightarrow 0 \]

But the limit of infinitely rigid particles can not be reached in this framework:

\[ \frac{p}{E} = 0 \quad !? \]
Contact Dynamics (CD)

Elastic force laws are required when a granular material is described as a multibody system with contact interactions.

But a granular material may also be viewed as a multicontact system governed by rigid-body dynamics.

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Kinematic constraints

1) Unilateral contact

\[
\begin{align*}
\delta_n > 0 & \implies f_n = 0 \\
\delta_n = 0 & \land \quad \begin{cases} 
    u_n > 0 & \implies f_n = 0 \\
    u_n = 0 & \implies f_n \geq 0
\end{cases}
\end{align*}
\]

0 \leq f_n \perp u_n \geq 0

Complementarity relation
II) Coulomb friction

\[
\begin{align*}
    u_t > 0 & \Rightarrow f_t = -\mu f_n \\
    u_t = 0 & \Rightarrow -\mu f_n \leq f_t \leq \mu f_n \\
    u_t < 0 & \Rightarrow f_t = \mu f_n
\end{align*}
\]

Complementarity relation

\[
\begin{align*}
    0 \leq \mu f_n + f_t & \perp u_t + |u_t| \geq 0 \\
    0 \leq \mu f_n - f_t & \perp -u_t + |u_t| \geq 0
\end{align*}
\]
Contact dynamics equations

Particle dynamics
\[ M(U^+ - U^-) = \delta t(F + F_{ext}) \]

Express dynamics in contact variables:
\[ u, \quad u_t, \quad f_n, \quad f_t \]

Since the contact velocities \( u \) are linear in particle velocities, the transformation of the velocities is an affine application.

\[ u = G U \quad G \quad 2N_c \times 3N_p \]

The transformation of the contact forces to force resultants is an affine application:

\[ F = H f \quad H = G^T \quad 3N_p \times 2N_c \]

\[ u^+ - u^- = \delta t H^T M^{-1} H f + \delta t H^T M^{-1} F_{ext} \]

Contact Dynamics Equations
The velocity involved in contact laws is a mean velocity weighted between the left-limit and right-limit velocities (observable velocities):

\[ u_n = \frac{u_n^+ + e_n u_n^-}{1 + e_n} \quad u_t = \frac{u_t^+ + e_t u_t^-}{1 + e_t} \]

\[
\frac{1 + e_n}{\delta t} \left( u_n^\alpha - u_n^{\alpha-} \right) = \mathcal{W}_{nn}^{\alpha\alpha} f_n + \mathcal{W}_{nt}^{\alpha\alpha} f_t \\
+ \sum_{\beta(\neq \alpha)} \{ \mathcal{W}_{nn}^{\alpha\beta} f_n + \mathcal{W}_{nt}^{\alpha\beta} f_t \} + \sum_{i,j} H^{T,\alpha i}_{n} M^{-1,ij} F_{ext}^j
\]

\[
\frac{1 + e_t}{\delta t} \left( u_t^\alpha - u_t^{\alpha-} \right) = \mathcal{W}_{tn}^{\alpha\alpha} f_n + \mathcal{W}_{tt}^{\alpha\alpha} f_t \\
+ \sum_{\beta(\neq \alpha)} \{ \mathcal{W}_{tn}^{\alpha\beta} f_n + \mathcal{W}_{nt}^{\alpha\beta} f_t \} + \sum_{i,j} H^{T,\alpha i}_{t} M^{-1,ij} F_{ext}^j
\]
\[ \mathcal{W}^{\alpha \beta}_{k_1 k_2} = \sum_{i,j} H^{T,\alpha i}_{k_1} M^{-1,ij} H^{j\beta}_{k_2} \]

\[ \mathcal{W}^{\alpha \alpha}_{nn} = \frac{1}{m_{1\alpha}} + \frac{1}{m_{2\alpha}} + \frac{(c_{1t}^\alpha)^2}{I_{1\alpha}} + \frac{(c_{2t}^\alpha)^2}{I_{2\alpha}} \]

\[ \mathcal{W}^{\alpha \alpha}_{tt} = \frac{1}{m_{1\alpha}} + \frac{1}{m_{2\alpha}} + \frac{(c_{1n}^\alpha)^2}{I_{1\alpha}} + \frac{(c_{2n}^\alpha)^2}{I_{2\alpha}} \]

\[ \mathcal{W}^{\alpha \alpha}_{nt} = \mathcal{W}^{\alpha \alpha}_{tn} = \frac{c_{1n}^\alpha c_{1t}^\alpha}{I_{1\alpha}} + \frac{c_{2n}^\alpha c_{2t}^\alpha}{I_{2\alpha}} \]

with

\[ c_{in}^\alpha = \vec{c}_i^\alpha \cdot \vec{n}^\alpha \]

\[ c_{it}^\alpha = \vec{c}_i^\alpha \cdot \vec{t}^\alpha \]
Alternative representation:

\[
\mathcal{W}_{nn} \alpha \alpha f_n^\alpha + \mathcal{W}_{nt} \alpha \alpha f_t^\alpha = (1 + e_n) \frac{1}{\delta t} u_n^\alpha + a_n^\alpha
\]

\[
\mathcal{W}_{tt} \alpha \alpha f_t^\alpha + \mathcal{W}_{tn} \alpha \alpha f_n^\alpha = (1 + e_t) \frac{1}{\delta t} u_t^\alpha + a_t^\alpha
\]

with

\[
a_n^\alpha = b_n^\alpha - (1 + e_n) \frac{1}{\delta t} u_n^{\alpha-} + \left( \frac{\vec{F}_{2a}^{\alpha}}{m_{2\alpha}} - \frac{\vec{F}_{1a}^{\alpha}}{m_{1\alpha}} \right) \cdot \vec{n}^\alpha
\]

\[
a_t^\alpha = b_t^\alpha - (1 + e_t) \frac{1}{\delta t} u_t^{\alpha-} + \left( \frac{\vec{F}_{2a}^{\alpha}}{m_{2\alpha}} - \frac{\vec{F}_{1a}^{\alpha}}{m_{1\alpha}} \right) \cdot \vec{t}^\alpha
\]

and

\[
b_n^\alpha = \frac{1}{m_{2\alpha}} \sum_{\beta(\neq \alpha)} \vec{f}_{2\alpha}^\beta \cdot \vec{n}^\alpha - \frac{1}{m_{1\alpha}} \sum_{\beta(\neq \alpha)} \vec{f}_{1\alpha}^\beta \cdot \vec{n}^\alpha
\]

\[
b_t^\alpha = \frac{1}{m_{2\alpha}} \sum_{\beta(\neq \alpha)} \vec{f}_{2\alpha}^\beta \cdot \vec{t}^\alpha - \frac{1}{m_{1\alpha}} \sum_{\beta(\neq \alpha)} \vec{f}_{1\alpha}^\beta \cdot \vec{t}^\alpha
\]
Iterative resolution

In order to solve the system of contact dynamics equations with the corresponding complementarity relations, we proceed by an iterative method which converges to the solution simultaneously for all contact forces and velocities.
Nonsmooth Mechanics

The Contact Dynamics method was formulated by Jean Jacques Moreau in 1988 in the framework of Nonsmooth Analysis and in terms of subdifferentials introduced by him in 1962.


Rough incline made of fixed grains
Friction: 0.3 everywhere
Slope: 29°

Polygonal grains of random shapes

J. J. Moreau, 1996
NonSmooth Analysis (NSA)

- Derivative
- Gradient
- Chebyshev polynomials
- Directional derivative
- Subdifferential of convex functions (introduced in 1962 by J.J. Moreau)
Back to rheology

CD simulations of simple shear with bi-periodic boundary conditions.

\[ q = \frac{1}{2}(\sigma_1 - \sigma_2) \quad p = \frac{1}{2}(\sigma_1 + \sigma_2) \]

\( \nu \) packing fraction

\( q/p \)

\( \rho \) packing fraction

(a) dense

(b) loose
Stress-dilatancy relationship

\[ \sin \varphi = \sin \varphi_c + \sin \psi \]
A graph shows a relationship between two variables, with axes labeled $z$ and $a$. The graph includes legend entries for 'loose +', 'dense +', 'cyclic', and 'reverse'. The data points are scattered across the plot, indicating a complex relationship between the variables.
**Fabric states**

A simple model based on the fabric parameters: \( \{ z, a_c, \theta_c \} \)

\[
E(\theta) = \frac{z}{2\pi} \{ 1 + a_c \cos 2(\theta - \theta_c) \}
\]

Steric exclusions \( \rightarrow \) upper bound: \( z \leq z_{\text{max}} \)

Mechanical equilibrium \( \rightarrow \) lower bound: \( z_{\text{min}} \leq z \)

\( \Rightarrow \) Two limit states:

1) Loosest isotropic state:
   \[
   E_{\text{max}} = \frac{z_{\text{max}}}{2\pi}
   \]

2) Densest isotropic state:
   \[
   E_{\text{min}} = \frac{z_{\text{min}}}{2\pi}
   \]
Assumption: all other states are enclosed between the two limit isotropic states

\[ E_{\text{min}} \leq E \leq E_{\text{max}} \]
Upper bound on the anisotropy as a function of $\mathcal{Z}$

$$a_c^{max}(\mathcal{Z}) = 2\min \left\{ 1 - \frac{\mathcal{Z}^{min}}{\mathcal{Z}}, \frac{\mathcal{Z}^{max}}{\mathcal{Z}} - 1 \right\}$$
\[ a_c^* = a_c^{\text{max}}(z^*) = \frac{2a_c^{\text{max}} - a_c^{\text{min}}}{a_c^{\text{max}} + a_c^{\text{min}}} \]

\[ z^* = \frac{z^{\text{min}} + z^{\text{max}}}{2} \]

Inertial critical states

\[ \dot{\varepsilon}_q \quad \text{shear rate} \]

\[ \rho \quad \text{mean stress} \]

\[ v \sim \dot{\varepsilon}_q d \quad \text{typical collision velocity} \]

\[ f_d \sim m v \times \dot{\varepsilon}_q^{-1} = m d \dot{\varepsilon}_q^2 \quad \text{typical impulsive force} \]

\[ f_s = p d^2 \quad \text{typical static force} \]

\[ I = \sqrt{\frac{f_d}{f_s}} = \dot{\varepsilon}_q \sqrt{\frac{m}{pd}} \quad \text{Inertial number} \]
\[ \mu = \tan \varphi^* \]
\[ \mu(I) = \mu_1 + \frac{\mu_2 - \mu_1}{1 + I_0/I} \]
\( e \sim -\log \left\{ \frac{p}{p_0} \right\} \)
\[
\frac{q}{p} = \sin \varphi = \frac{1}{2} (a_c + a_n + a_t)
\]
Cohesive critical states

Adhesion: The complementarity relations are shifted.

\[ f_n = -f_a \]

\[ \mu_s (f_n + f_a) \]

\[ f_t = -\mu_s (f_n + f_a) \]

\[ \eta = \frac{f_a}{pd} \]  

(2D)
Fit Eq (5)

\[
\frac{q}{p} = \sin \varphi + \frac{c}{p} \cos \varphi \\
\frac{c(I = 0)}{p} \sim \eta
\]
Modified inertial number

\[ f_s = pd + \alpha f_a \quad \Rightarrow \quad I_c = \frac{I}{(1 + \alpha \eta)^{1/2}} \]
\[ \frac{q}{p} \]

\[ \eta = 0 \]
\[ \eta = 5 \]
\[ \eta = 10 \]
\[ \eta = 15 \]
\[ \eta = 20 \]
Conclusion

The Contact Dynamics approach provides a general framework for the simulation of plastic deformations of granular materials.

The rheological behavior is reproduced without elastic force laws, thus indicating that the behavior is independent of elastic force law.

The critical state is characterized by both its connectivity and anisotropy.

The critical state may be extended to inertial and cohesive materials. The effect of adhesion is similar to that of particle inertia. Both parameters lead to reduced solid fraction and enhanced shear strength.