Constitutive behavior and numerical methods

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Outline

Introduction

Constitutive framework

Grain geometry

Contact interactions

Nonsmooth motion

Multibody dynamics

Molecular Dynamics method

Contact Dynamics Method

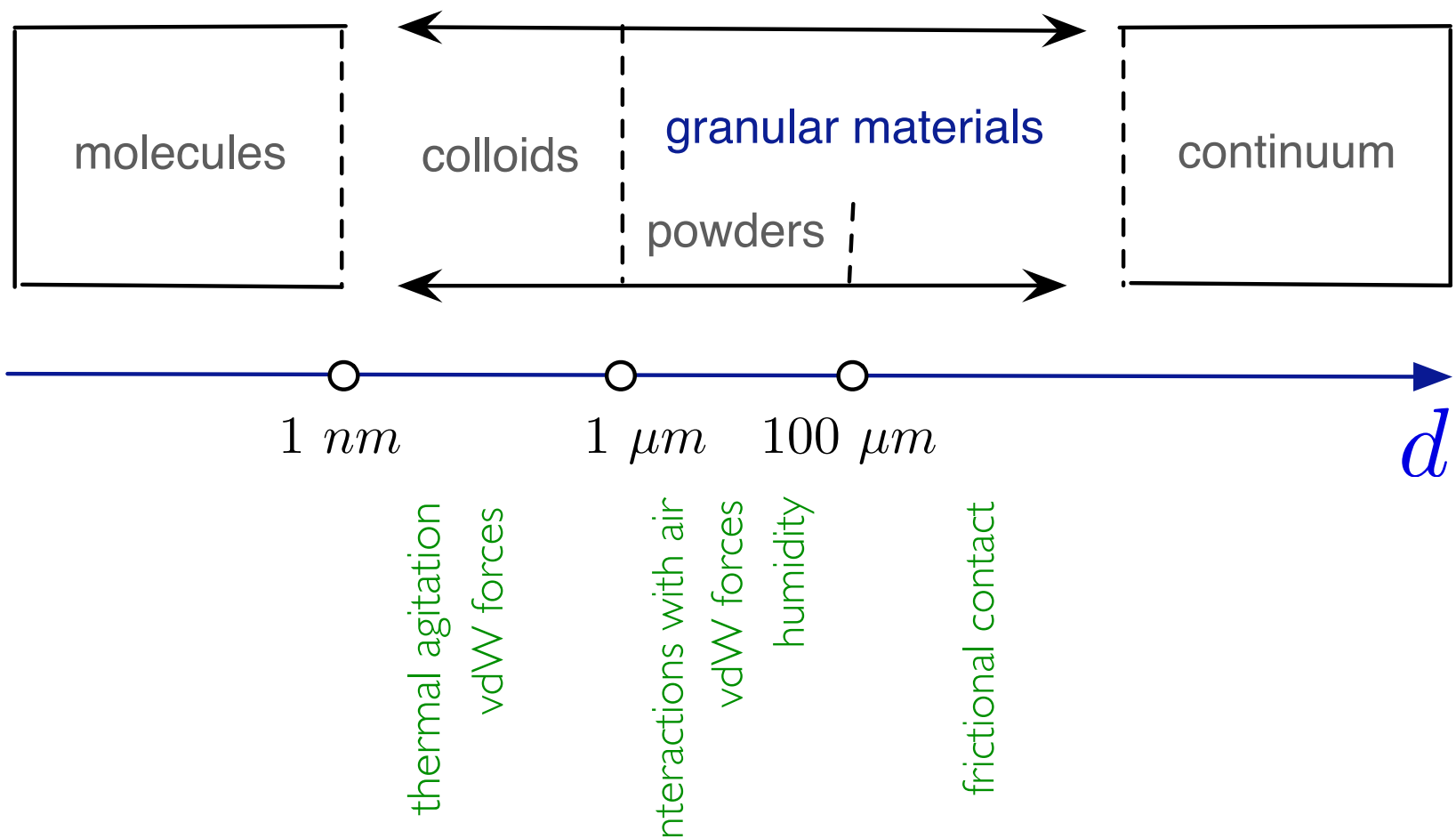
Extensions

Introduction

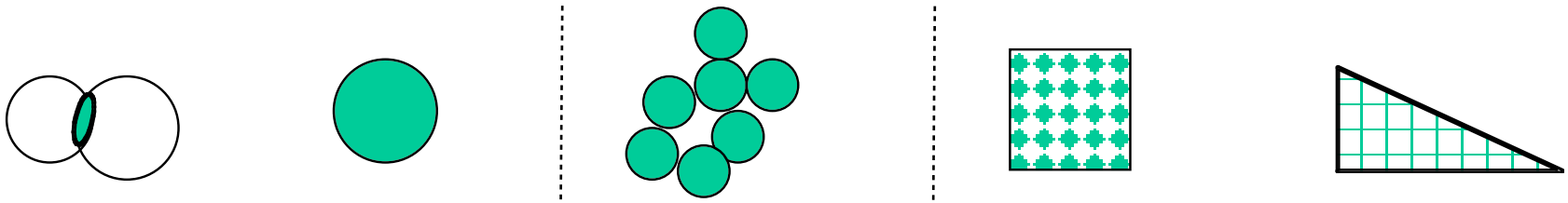
Granular materials: Collection of solid particles of size above $1\ \mu m$

➡ The interactions between particles are governed by frictional contact and inelastic collisions.

Granular materials



Multi-scale modeling



Contact δ | Particle d | Packing $g(r)$ | Material RVE | Structure, process BVP

scales of description

composition + interactions **Statistical behavior** **Constitutive behavior (rheology)**

DEM **FEM**

BVP: Boundary Value Problem

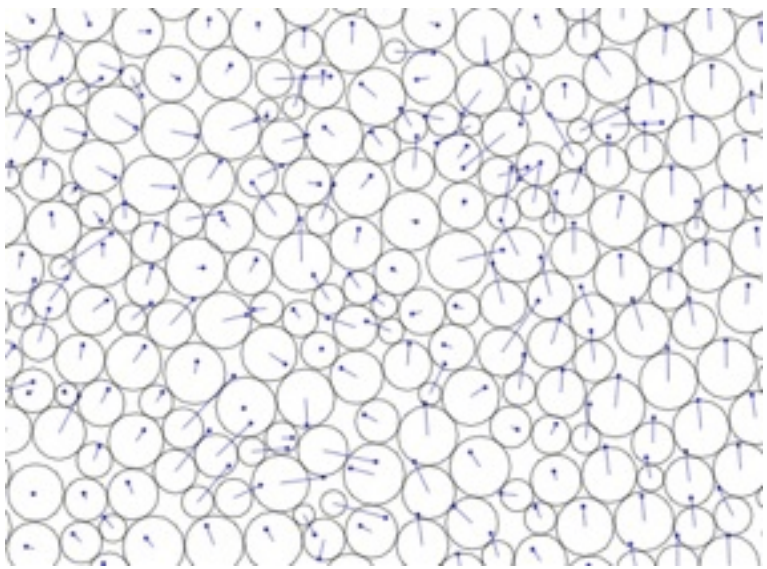
RVE: Representative Elementary Volume

DEM: Discrete Element Method

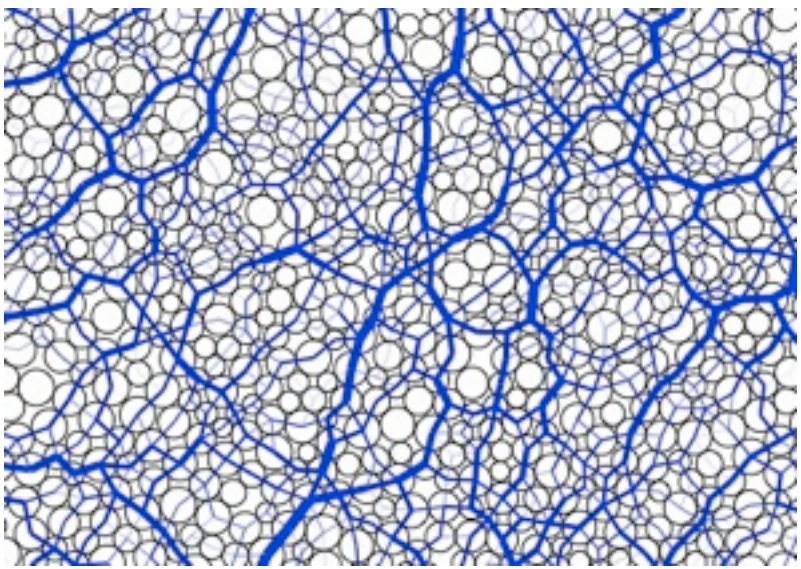
FEM: Finite Element Method

Granular materials are inhomogeneous at all scales:

1) Sub-RVE inhomogeneities arise from geometrical disorder.



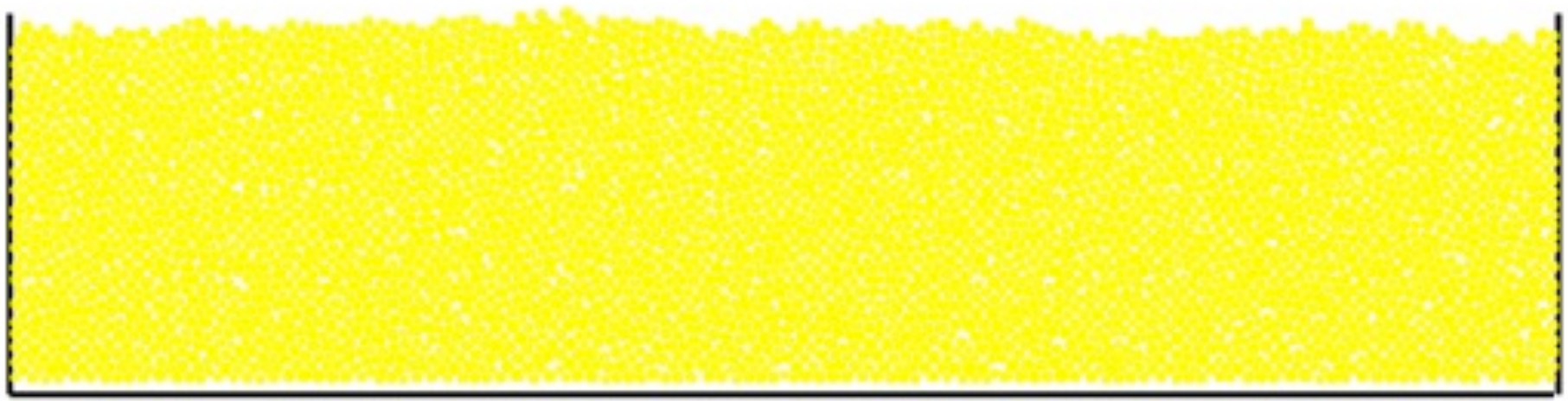
Particle velocities



Contact forces

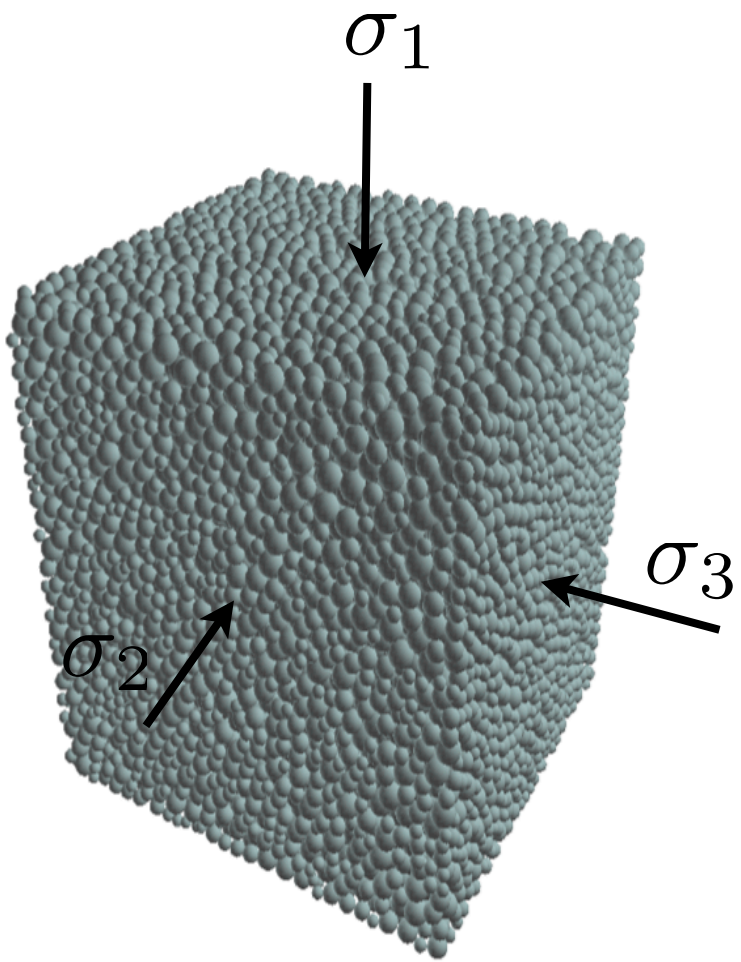
2) Large-scale inhomogeneities arise from bulk forces and complex boundary conditions.

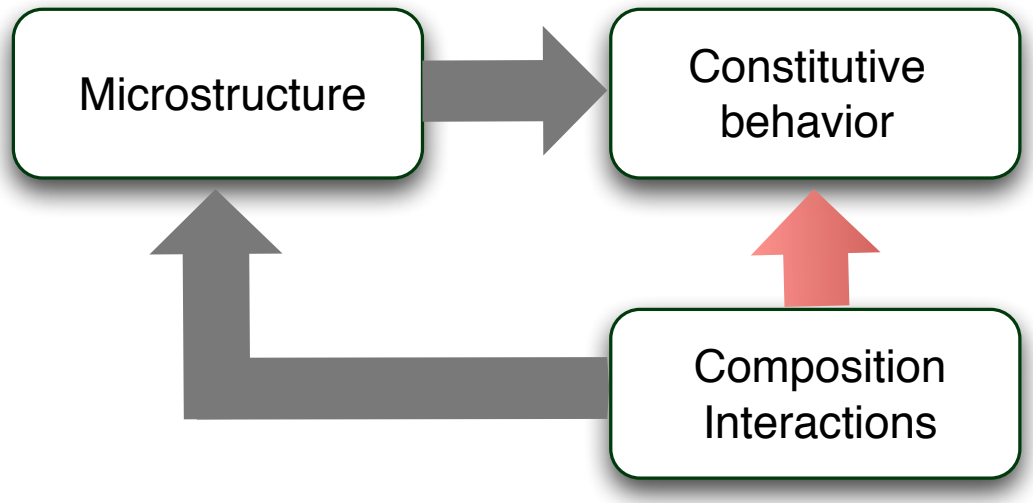
Inhomogeneities



Avalanche (by L. Staron)

The behavior is homogeneous when the strains and stresses are uniform in the bulk. This happens if the number of particles is large enough for the sample to be statistically representative and the finite-size and wall effects are absent. The sample may then be considered as a RVE and the behavior as intrinsic to the material (rheology).



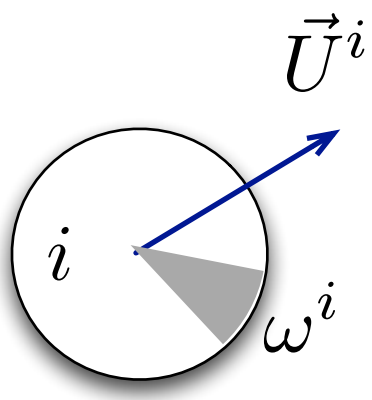


The homogeneous behavior is consequence of the composition and nature of interactions (example: frictional behavior). But these are mainly expressed at the macroscopic scale through the microstructure, which is at the origin of the emergent (generic, collective) properties of granular materials (example: internal friction angle evolves with the fabric anisotropy). Some properties are of purely structural nature (example: dilatancy).

The DEM provides a general tool for the investigation of the constitutive behavior by integrating the equations of motions of all particles, described by their geometrical and mechanical properties as well as their frictional interactions.

The DEM was introduced by Peter Cundall in 1975 by analogy ith the molecular dynamics method (MD), but applied to solid particles with frictional contacts. A radically different method, called contact dynamics (CD) was introduced in 1991 by Jean Jacques Moreau and Michel Jean.

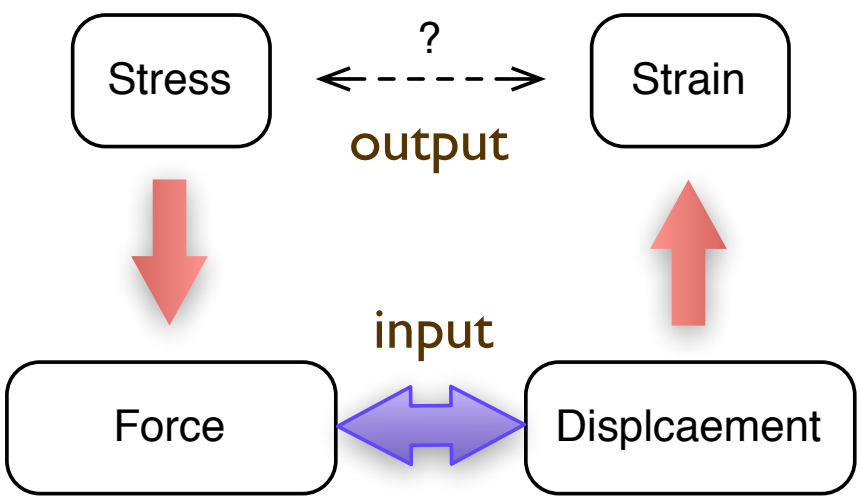
Their common feature is to describe the particles as rigid bodies with a finite number of degrees of freedom (dynamical variables): 6 in 3D and 3 in 2D.



Analogy with homogenization (coarse-graining, upscaling):

The physical input in both the DEM and homogenization is the composition and local interactions, and the macroscopic behavior is obtained from collective particle dynamics by averaging.

By providing detailed information about the microstructure and its evolution, the DEM is an ideal ally for analytical homogenization.



3 levels of discrete modeling:

1) Basic

Spherical particles + frictional contact interactions

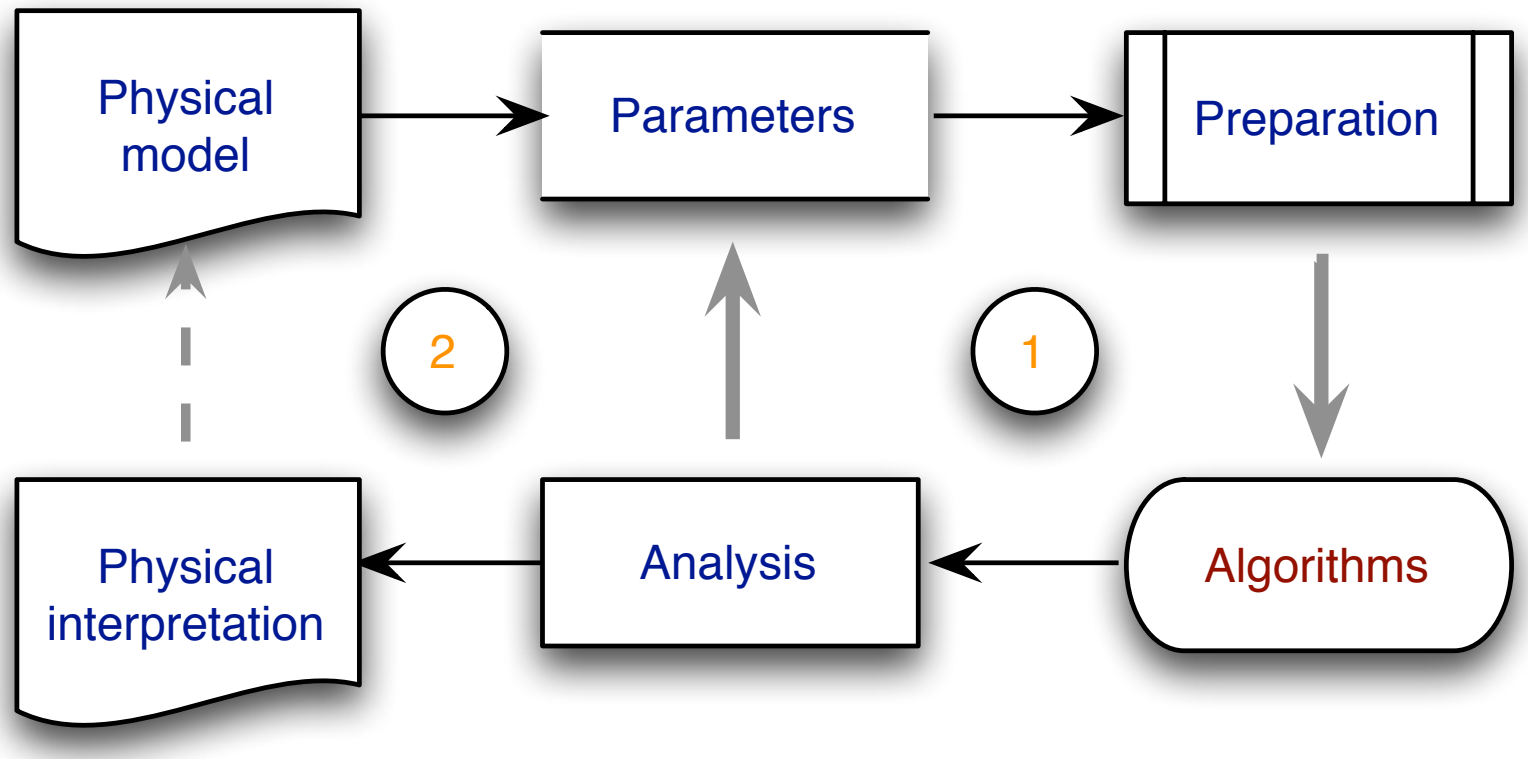
2) Extended

Particle clusters, adhesion forces (capillary, lubrication, adhesion threshold), high polydispersity, rolling friction

3) Advanced

Non-spherical particles, Particle fracture, pore-filling continuous phase (liquid, solid), evolving interactions and phase transformations

Modeling cycle



A physical model is defined by the choice of composition and paricle interactions. The model parameters need to be fixed and the initial state generated by a preparation method. The algorithm provides the evolution of particle positions. The numerical data are analyzed by post-processing. It might be necessary to adjust model parameters (cycle 1). If the physical interpretation is not consistent with the experimental behavior, the physical model should be modified (cycle 2).

Constitutive framework

elastic behavior

At very small strains, the behavior is elastic. The nonlinear behavior is a consequence of nonlinear Hertz law and the evolution of the number of contacts (see the coarse of J.-N. Roux).

plastic behavior

At very larger strains, the behavior is plastic. It is characterized by three ingredients:

1) Yield function (accessible stresses)
2) Flow rule (direction of plastic strain)
3) Hardening rule (evolution of the state parameters)

In the case of a granular material composed of rigid particles interacting via a Coulombic friction:

- No force scale → The yield surface in the stress space is expressed as a stress ratio → Coulomb cone →

Internal angle of friction φ

- The plastic strain reflects only the relative particle displacements + rate-independence →The volume change scales with the shear strain → flow rule given by an angle

Dilation angle ψ

Set of state parameters $\mathcal{F}$

$\Rightarrow$ The plastic behavior is defined by specifying

$$\varphi(\mathcal{F})$$
$$\psi(\mathcal{F})$$
$$\dot{\mathcal{F}}(\mathcal{F}, \dot{\varepsilon})$$

Steady state:

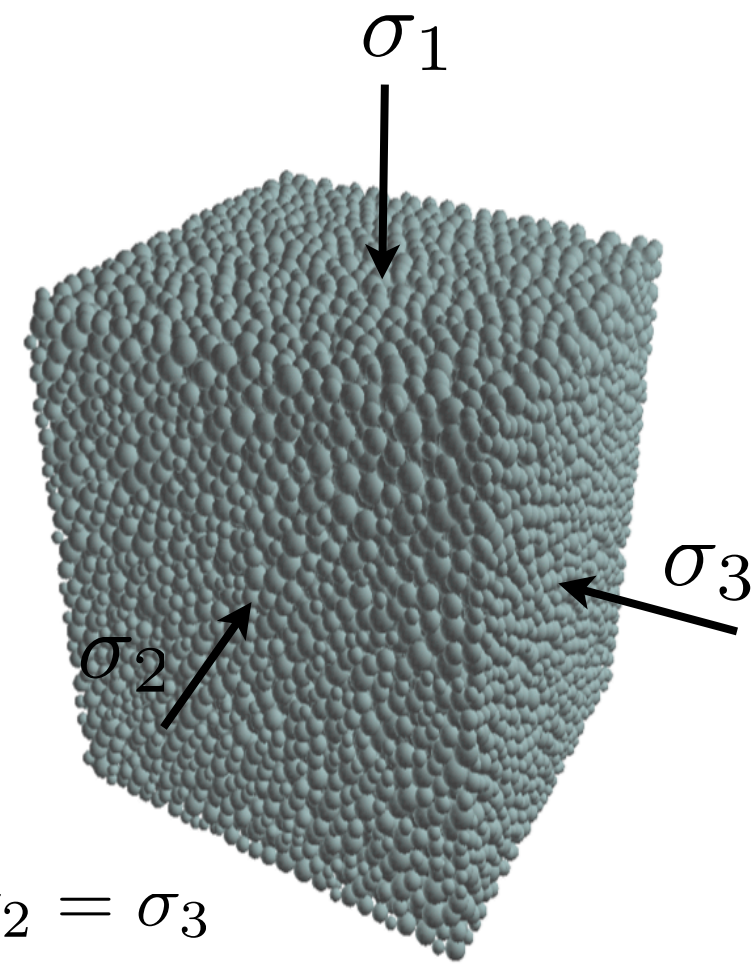
$$\varphi^* = \varphi(\mathcal{F}^*)$$
$$\psi^* = \psi(\mathcal{F}^*) = 0$$

Angle of friction in terms of stress invariants:

$$p = \frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3)$$

3D $$q = \frac{1}{3}(\sigma_1 - \sigma_3)$$

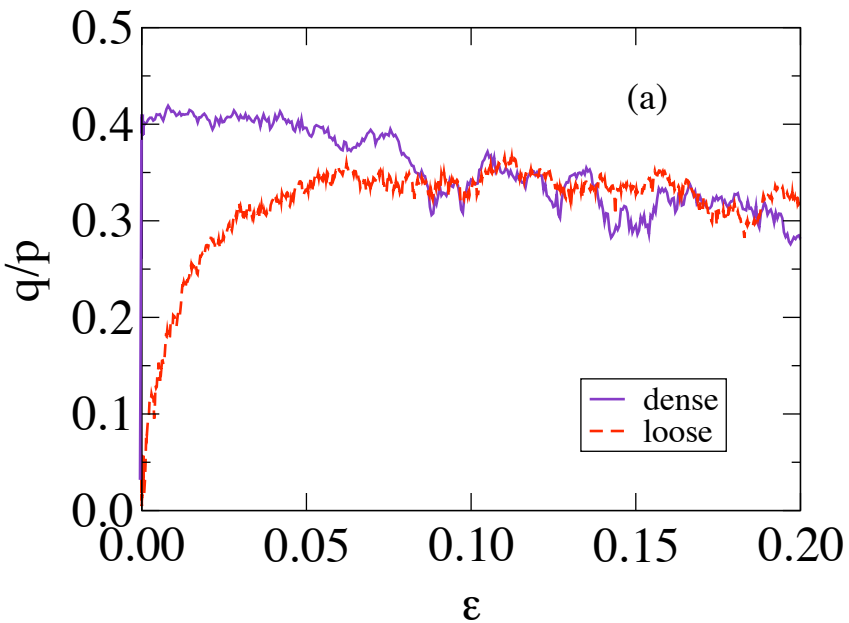
$$\Rightarrow \quad \sin\varphi = \frac{3q}{2p+q}$$

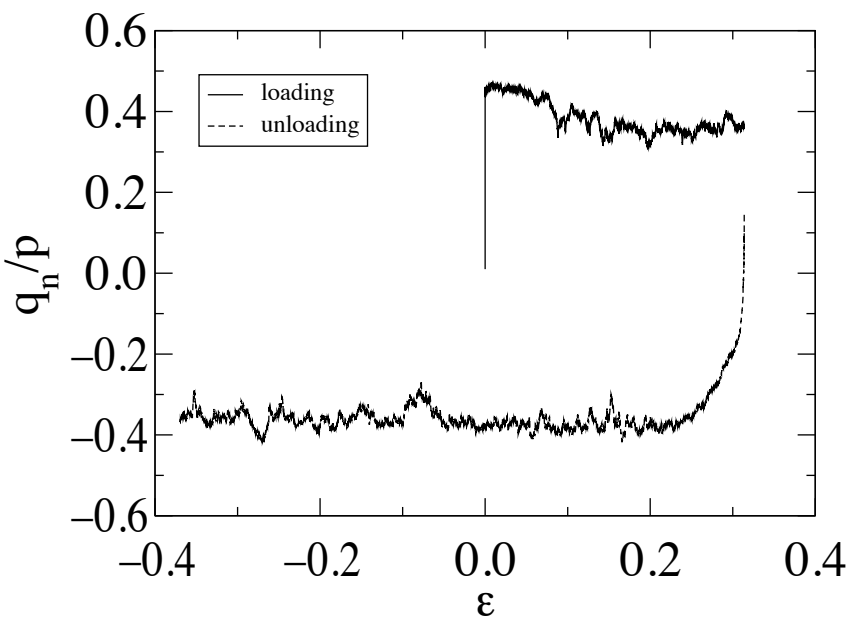


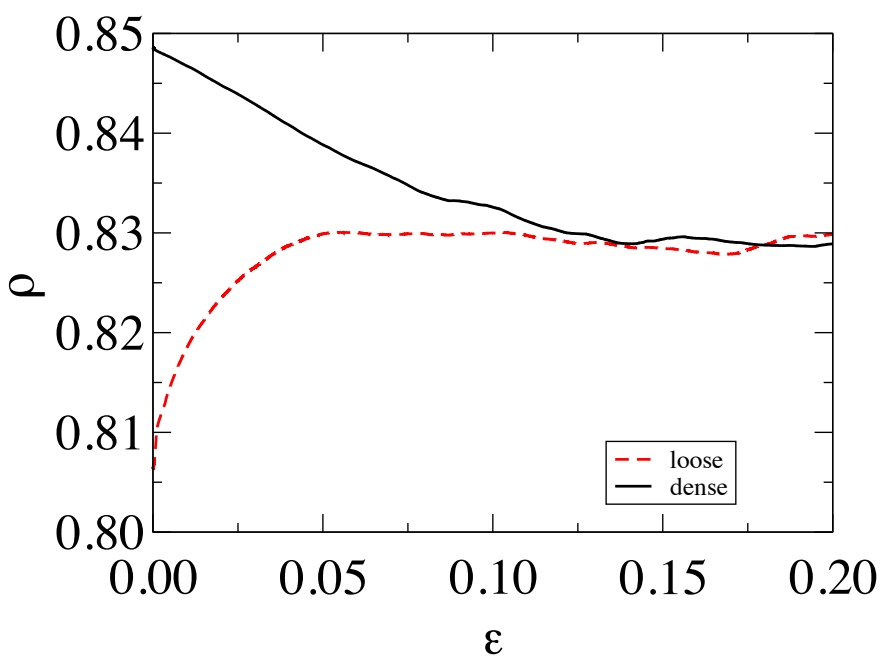
$$p = \frac{1}{2}(\sigma_1 + \sigma_2)$$

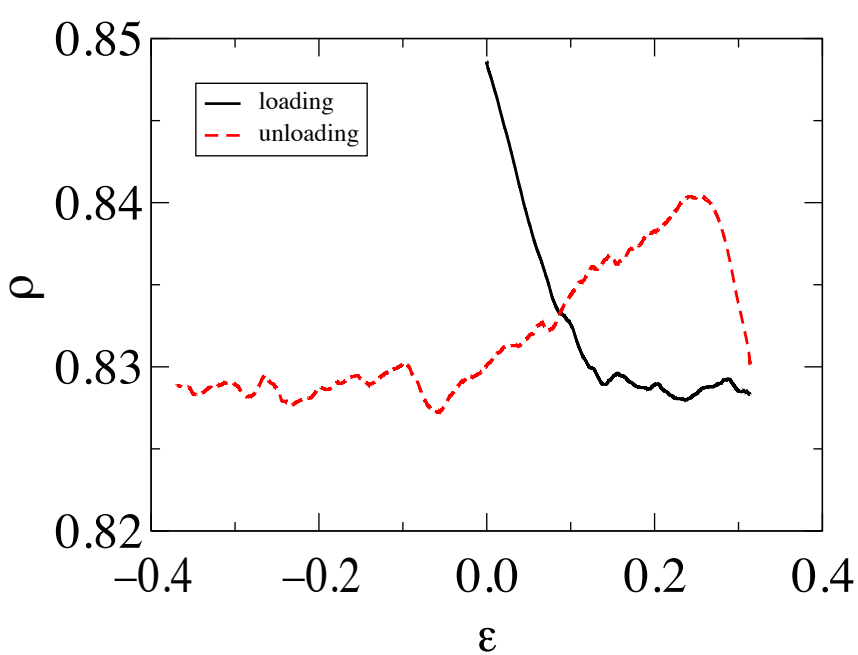
2D $$q = \frac{1}{2}(\sigma_1 - \sigma_2)$$

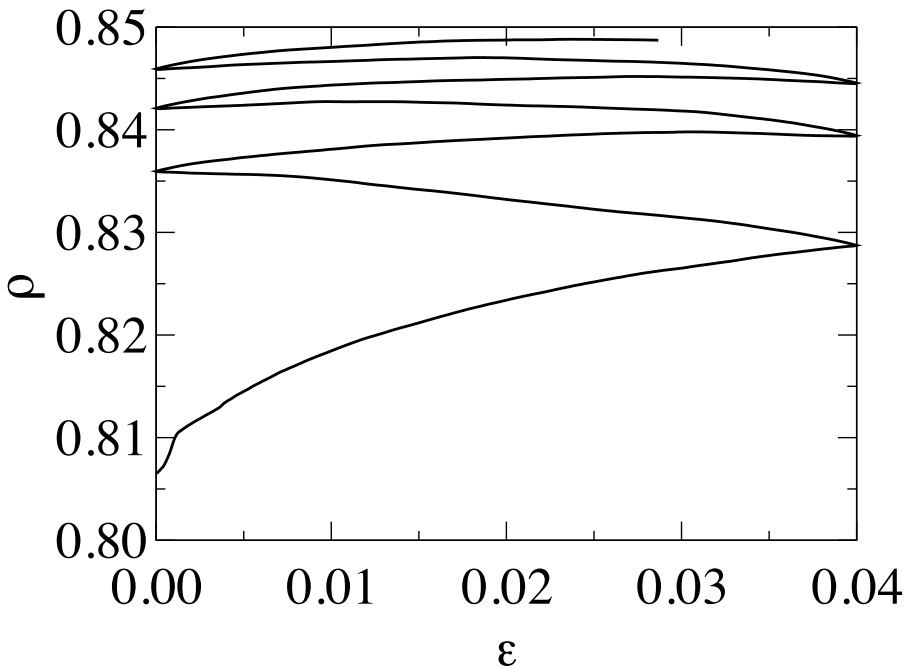
$$\Rightarrow \quad \sin\varphi = \frac{q}{p} \qquad \sigma_2 = \sigma_3$$


(a)
q/p
ε
dense
loose

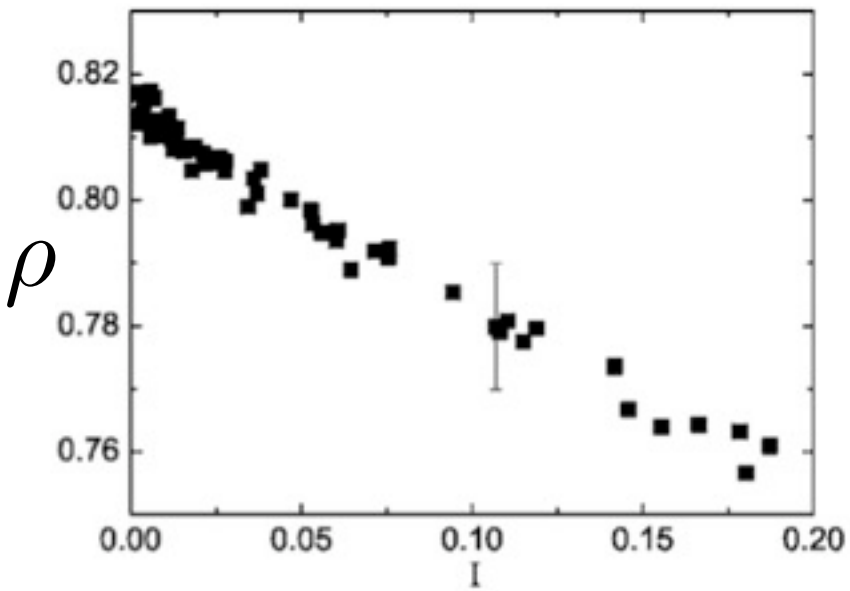

q_n/p
ε
loading
unloading


ρ
ε
loose
dense


ρ
ε
loading
unloading

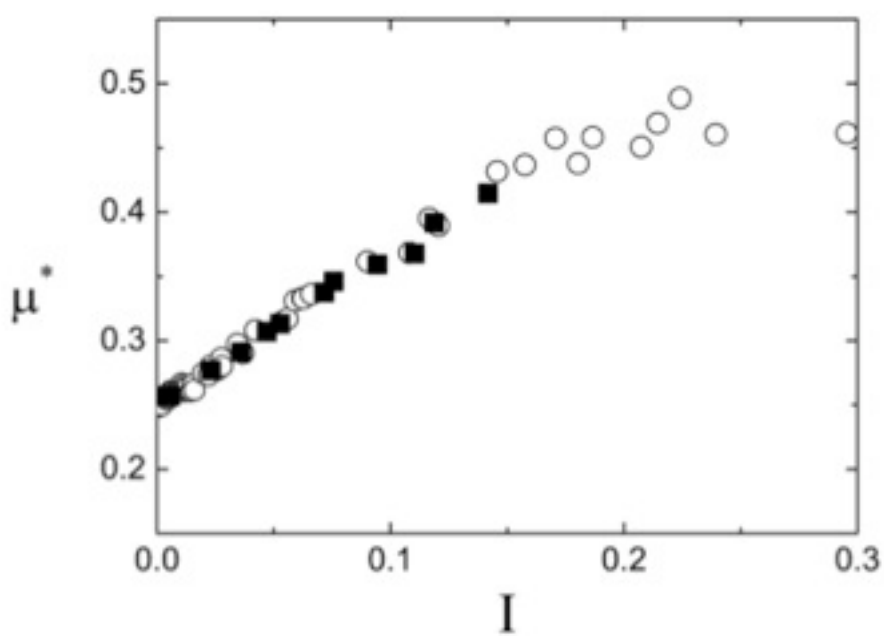

0.85
0.84
0.83
0.82
0.81
0.80
ρ
0.00
0.01
0.02
0.03
0.04
ε

viscous behavior at large strain-rates



$$\rho(I) \simeq \rho_{max} - a\ I$$

$$I = \dot{\varepsilon}\sqrt{\frac{m}{pd}}$$

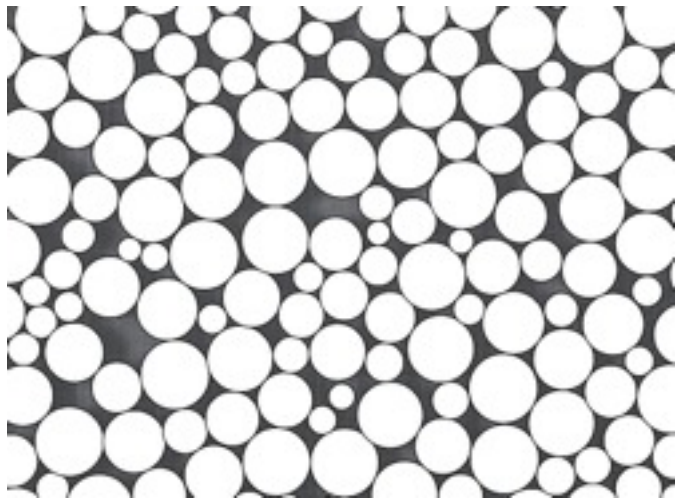


$$\mu^*(I) \simeq \mu_{min} + b\ I$$

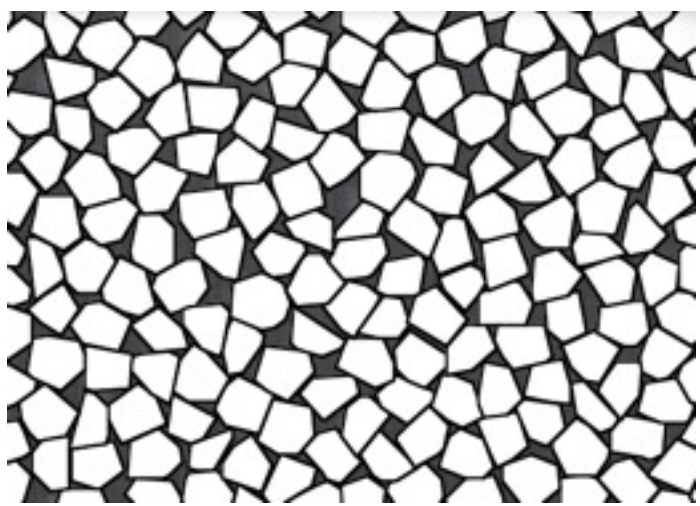
Grain geometry

Polydispersity

Size polydispersity



Shape polydispersity



Size polydispersity

Definitions

$f(d)$ Proportion of grains with diameter d

$V(d)$ Volume fraction of grains of size d

$F(d)$ Proportion of grains of size below d

$h(d)$ Cumulative volume fraction of grains

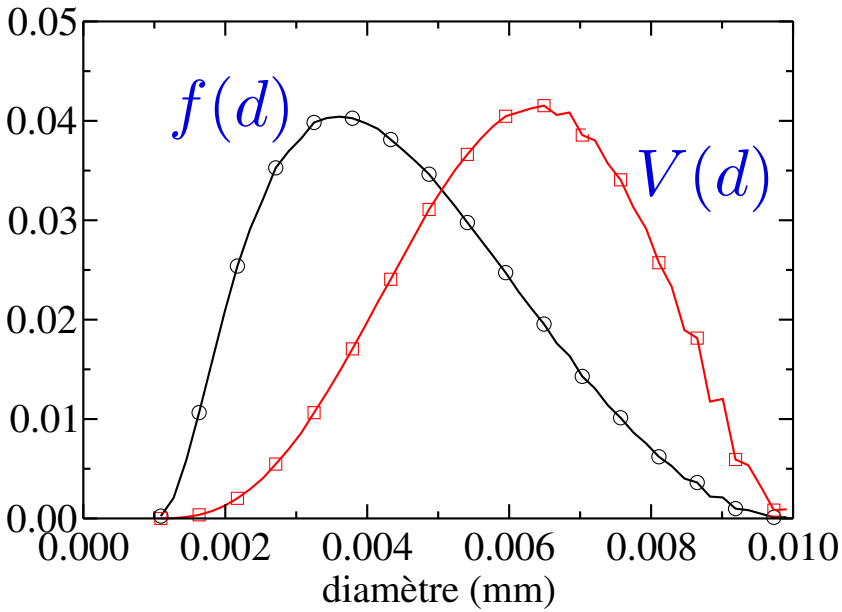
Grading curve

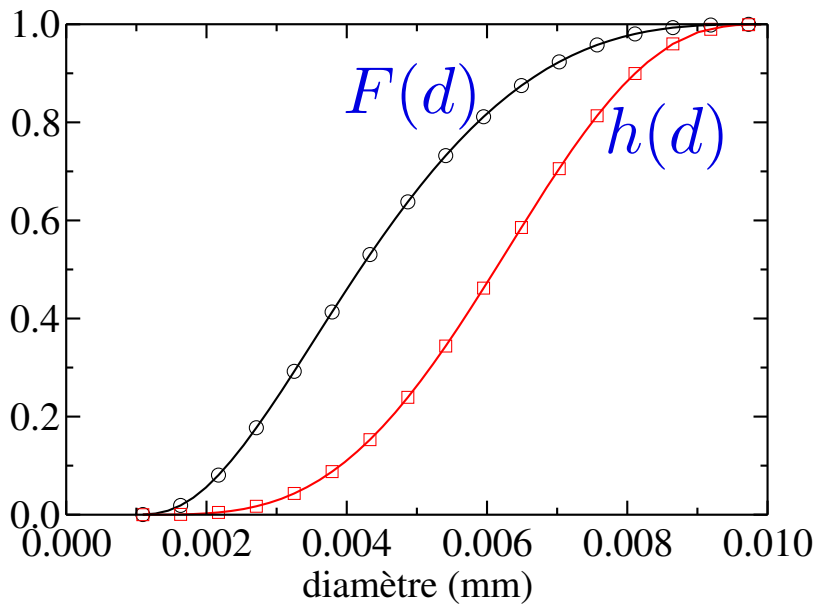
$$F(d) = \int_{d_{min}}^{d} f(x)\ dx \qquad h(d) = \frac{\int_{d_{min}}^{d} V(x)f(x)dx}{\int_{d_{min}}^{d_{max}} V(x)f(x)dx}$$

d_{min} **lower bound**

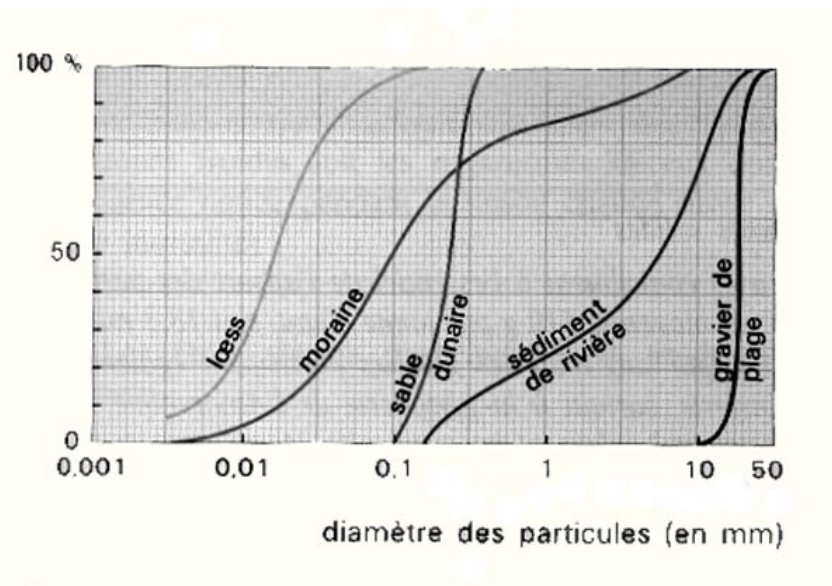
d_{max} **upper bound**

Example

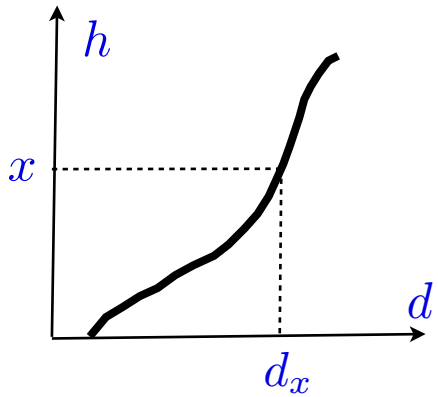




Grading curve



$$d_x = h^{-1}(x)$$



$$C_u = \frac{d_{60}}{d_{10}}$$ **Coefficient of uniformity**

$$C_c = \frac{d_{30}^2}{d_{10} d_{60}}$$ **Coefficient of curvature**

$$d_{60} - d_{10}$$ **Size span**

Mono-disperse system $C_u = 1$

d_{min}

d_{max}

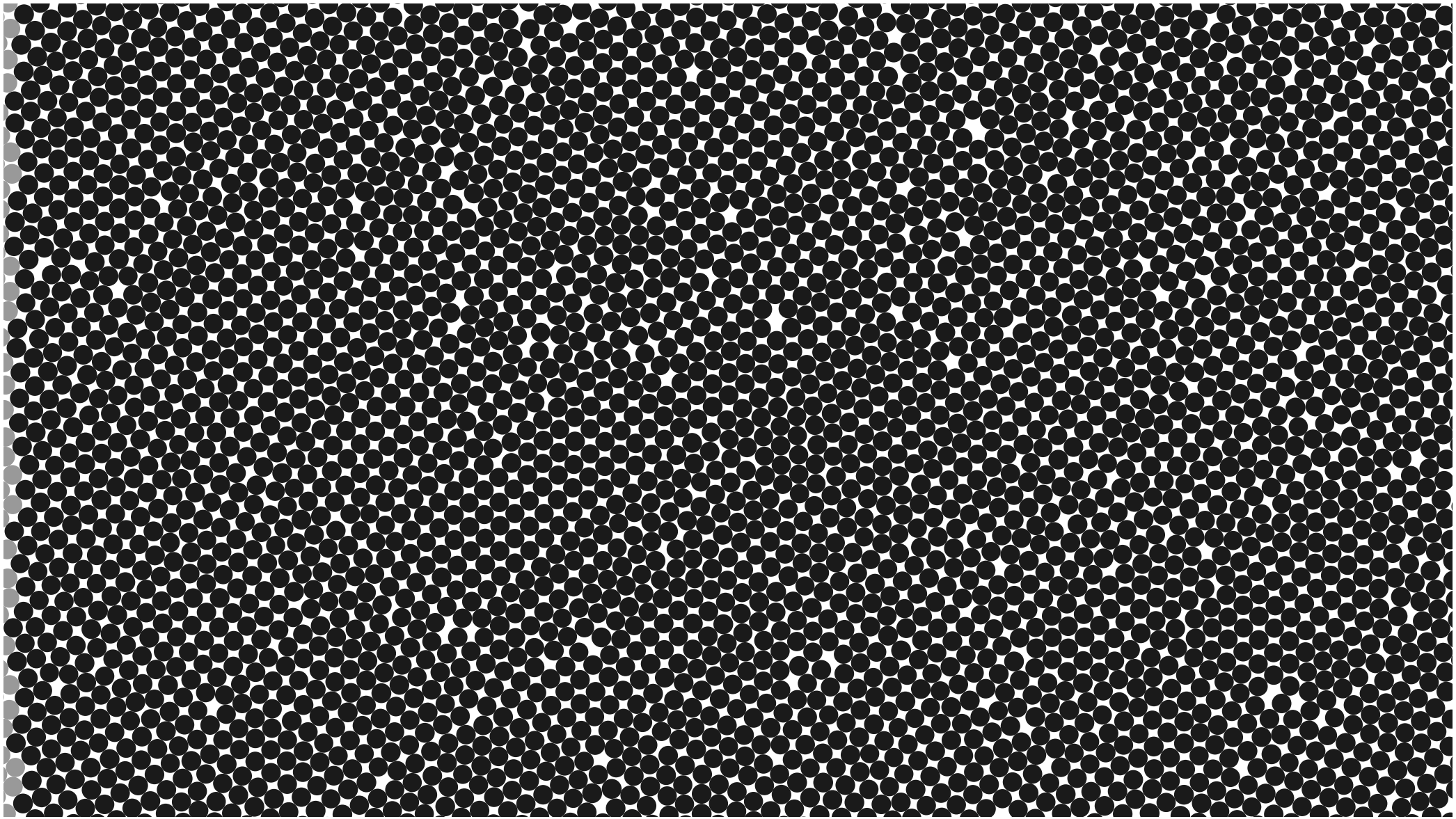
$$d_r(d) = \frac{d - d_{min}}{d_{max} - d_{min}}$$ **reduced size**

$$s = \frac{d_{max} - d_{min}}{d_{max} + d_{min}}$$ **span**

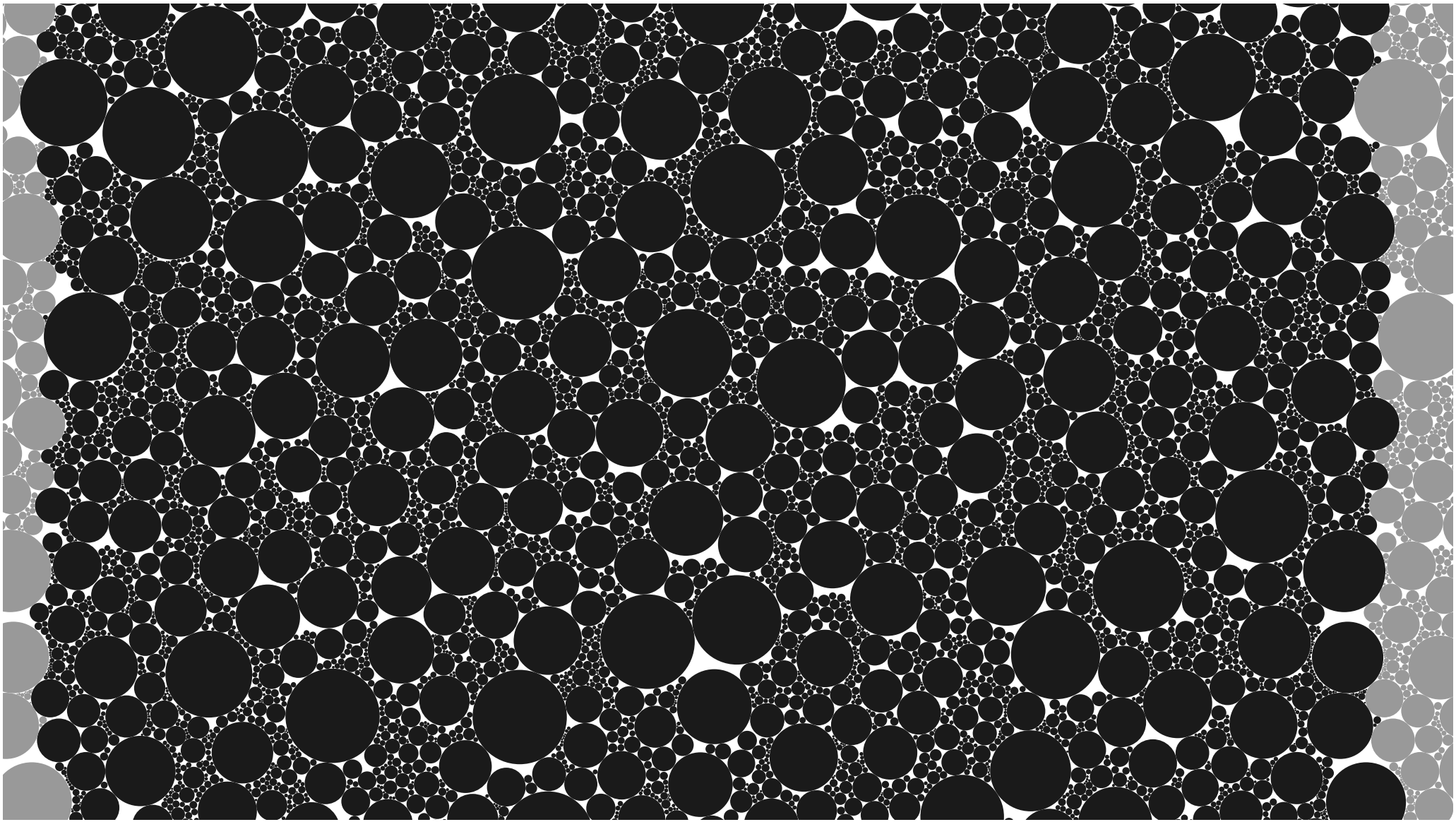
N_c Number of classes N_p Number of particles

$$\delta d = \frac{d_{max} - d_{min}}{N_c}$$

$N_p f(d)\ \delta d$ Number of grains of size $\in [d - \delta d/2, d + \delta d/2]$



$$s = 0.02$$

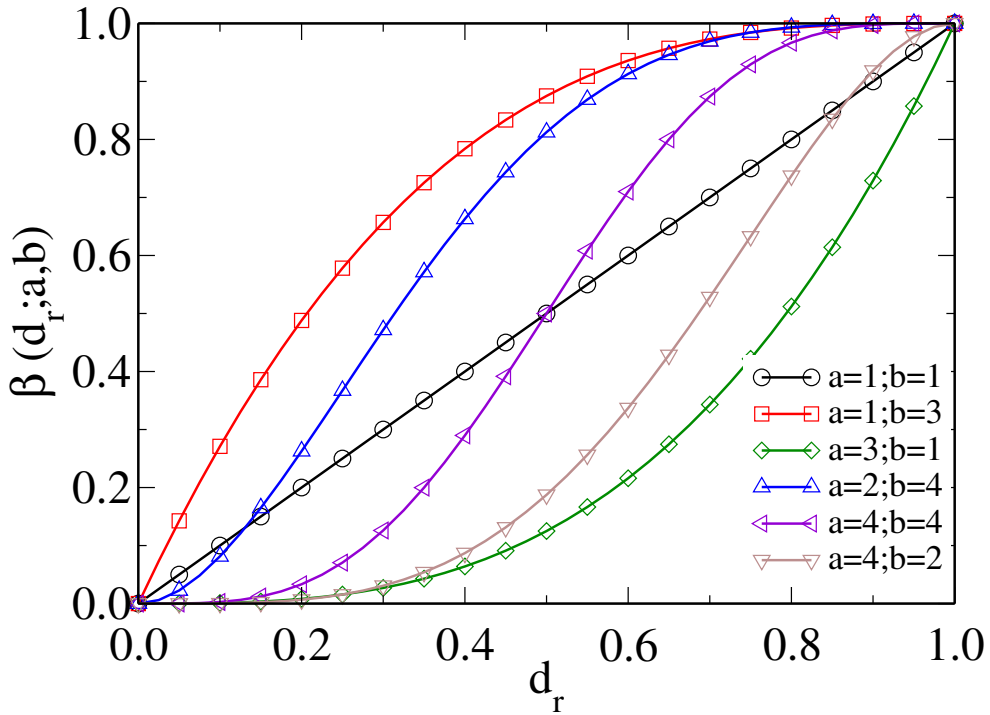


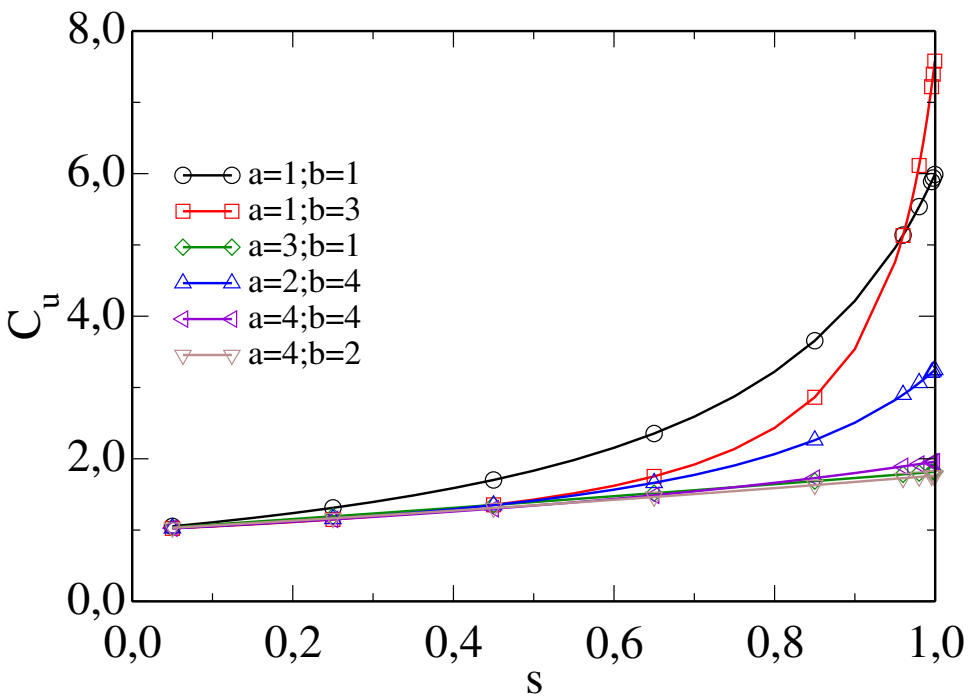
$$s = 0.97$$

The quality of the discretized grading function depends on

- the number of classes
- the number of grains in each class
- the volume of grains in each class

For the simulation of polydisperse systems, the tractable number of particles should be comprimized with the statistical representativity of the size distribution.


1.0
0.8
0.6
0.4
0.2
0.0
β (d_r;a,b)
0.0
0.2
0.4
0.6
0.8
1.0
d_r
a=1;b=1
a=1;b=3
a=3;b=1
a=2;b=4
a=4;b=4
a=4;b=2


8,0
6,0
4,0
2,0
0,0
C_u
0,0
0,2
0,4
0,6
0,8
1,0
s
a=1;b=1
a=1;b=3
a=3;b=1
a=2;b=4
a=4;b=4
a=4;b=2

Contact interactions

Granular dynamics involves fine length scales such as elastic particle deformations, contact deflection

λ sub-particle length scale (contact deformation, ...)

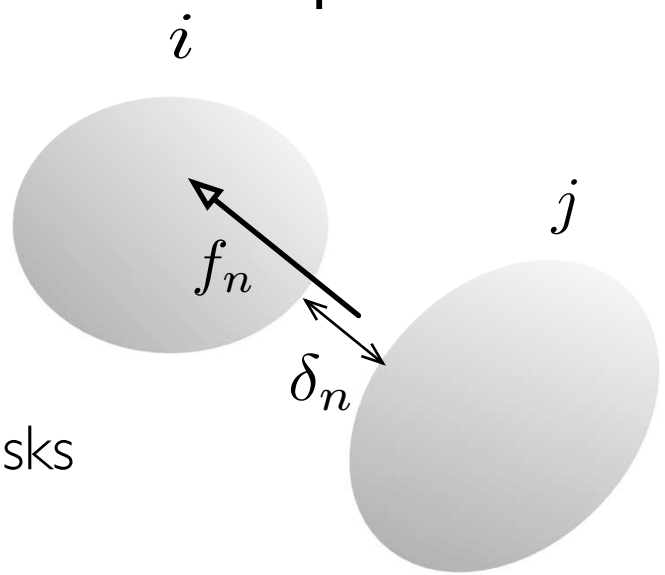
δr spatial resolution

length scales

$\delta r \gg \lambda$ $\Rightarrow$ The spatial resolution is too large to resolve fine length scales.

$\Rightarrow$ particle-scale dynamics (rigid particles)

In particle-scale dynamics, the contact between two particles becomes a unilateral constraint.



f_n normal force

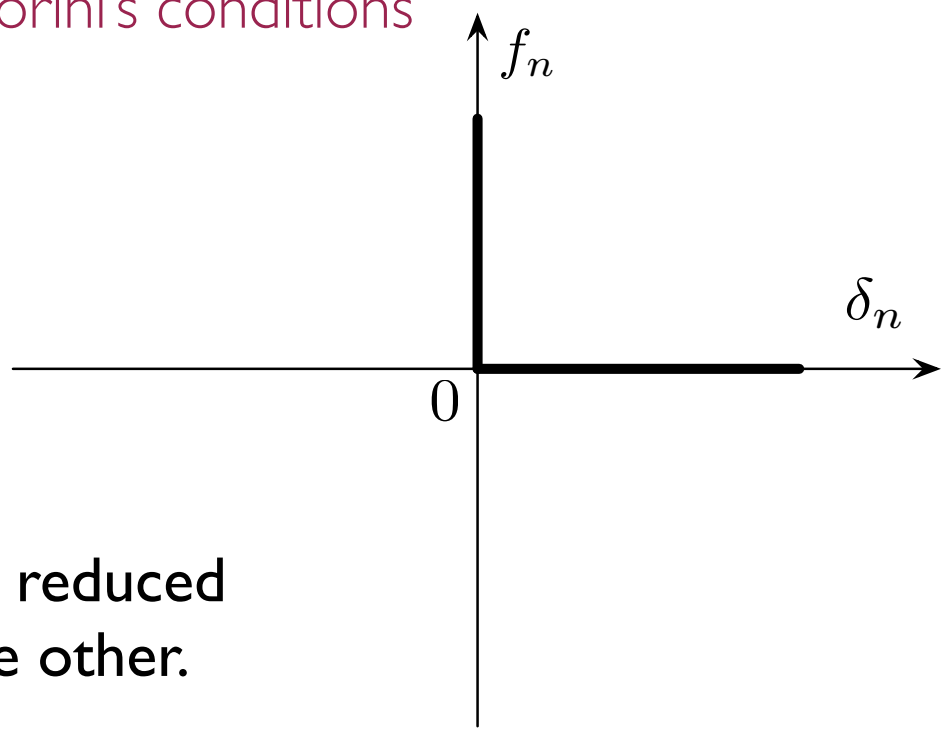
δ_n normal distance

$$\delta_n = \left|\mathbf{r}^i - \mathbf{r}^j\right| - a^i - a^j \quad \text{for two disks}$$

Signorini conditions

$$\begin{cases} \delta_n > 0 & \Rightarrow \quad f_n = 0 \\ \delta_n = 0 & \Rightarrow \quad f_n \geq 0. \end{cases}$$

Signorini's conditions



Alternative writing:

$$0 \leq f_n \quad \perp \quad \delta_n \geq 0$$

Complementarity relation

None of the two variables can be reduced to a (mono-valued) function of the other.

Persistent contact: $\delta_n = 0$ and $u_n = \dot{\delta}_n = 0$

Breaking contact: $\delta_n = 0$ and $u_n > 0$

The normal force vanishes at a breaking contact:

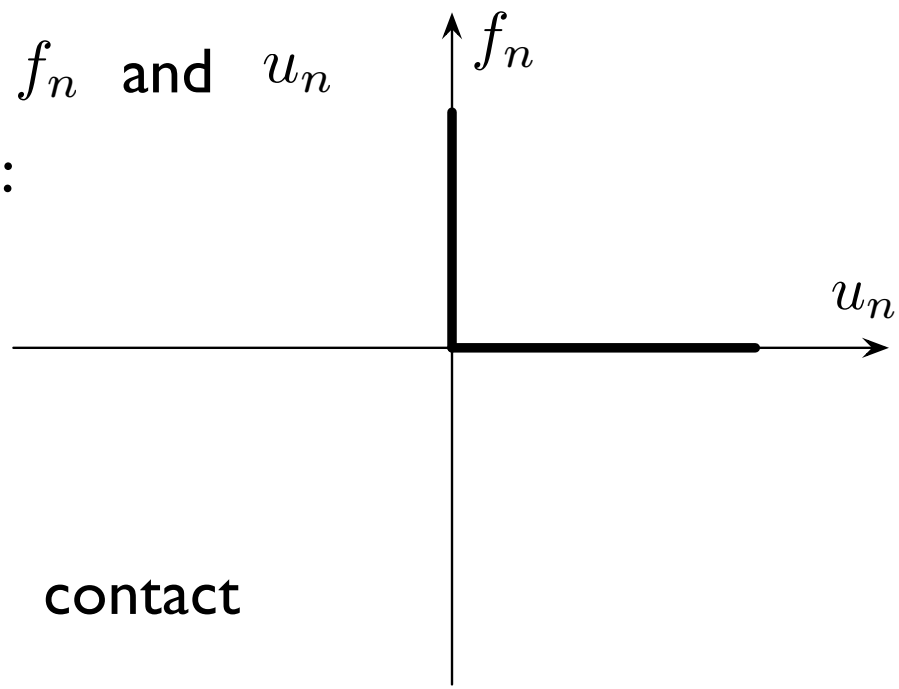
kinematic constraints

$$\begin{cases} \delta_n > 0 \quad \Rightarrow \quad f_n = 0 \\ \delta_n = 0 \quad \wedge \quad \begin{cases} u_n > 0 \quad \Rightarrow \quad f_n = 0 \\ u_n = 0 \quad \Rightarrow \quad f_n \geq 0 \end{cases} \end{cases}$$

$\Rightarrow$ for $\delta_n = 0$ (i.e. for a contact) f_n and u_n satisfy a complementarity relation:

$$0 \leq f_n \quad \perp \quad u_n \geq 0$$

velocity-Signorini conditions

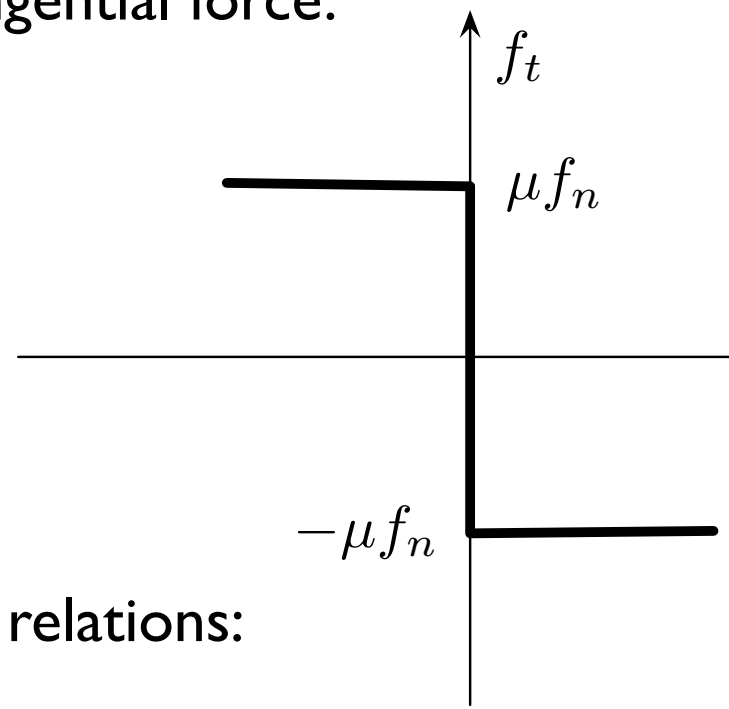


In this form, the geometrical contact becomes a kinematic constraint.

Coulomb friction law

The Coulomb law of dry friction is a nonsmooth relation between the sliding velocity and the tangential force.

$$\begin{cases} u_t > 0 & \Rightarrow & f_t = -\mu f_n \\ u_t = 0 & \Rightarrow & -\mu f_n \leq f_t \leq \mu f_n \\ u_t < 0 & \Rightarrow & f_t = \mu f_n \end{cases}$$



It can be cast in two complementarity relations:

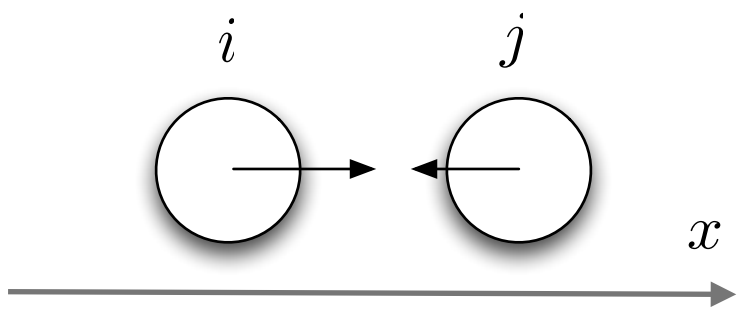
$$0 \leq \mu f_n + f_t \quad \perp \quad u_t + |u_t| \geq 0$$

$$0 \leq \mu f_n - f_t \quad \perp \quad -u_t + |u_t| \geq 0$$

Nonsmooth motion

Rigid-body dynamics is nonsmooth (involves velocity discontinuities).

Example: Head-on collision between two balls at time t



δt time resolution (time step)

τ contact duration

time scales

(1) $\delta t \ll \tau \quad \Rightarrow$ Smooth motion

The acceleration is defined: $\Gamma_x(t) = \dfrac{dU_x(t)}{dt}$

The motion is fully described by Newton's equations given the applied forces.

$$m^i \Gamma_x^i = F_x^i(t, r_x^i, U_x^i, r_x^j, U_x^j)$$

$$m^j \Gamma_x^j = F_x^j(t, r_x^i, U_x^i, r_x^j, U_x^j)$$

During collision and in the absence of external forces, we have

$$F_x^i = -F_x^j = f_x(r_x^i, U_x^i, r_x^j, U_x^j)$$

which is a material dependent force law.

(2) $\delta t \gg \tau$ $\Rightarrow$ Velocity jump $\delta U_x^i(t) = U_x^i(t+\delta t) - U_x^i(t)$

This is a "jump" in the sense that the velocity change occurs in negligibly small time. The time resolution is insufficient to resolve the motion.

Mathematically, this means that the velocity U_x^i has no density (is not differentiable) with respect to time.

$\Rightarrow$ In this mathematical limit, the acceleration is not defined.

$\Rightarrow$ The motion involves instantaneous velocity change:

left-limit velocity $U_x^{i-}(t)$ t $U_x^{i+}(t)$ right-limit velocity

The velocity jump replaces the acceleration:

$$\delta U_x^i(t) = U_x^{i+}(t) - U_x^{i-}(t)$$

Newton's equations should be "coarse-grained" by integration over the time resolution:

$$m(U_x^+ - U_x^-) = \int_{\delta t} F_x \, dt = P_x = \langle F_x \rangle \, \delta t$$

impulsion

time-averaged force

This relation simply expresses the conservation of linear momentum.

$$m^i(U_x^{i+} - U_x^{i-}) = P_x$$

For head-on collision:

$$m^j(U_x^{j+} - U_x^{j-}) = -P_x$$

These are 2 equations, but we have 3 unknowns:

$$P_x \qquad U_x^{i+} \qquad U_x^{j+}$$

For the description of nonsmooth motion (here, a collision), we need one more equation relating these variables.

Classically, the relative velocities before and after a collision event are related through a restitution coefficient:

$$U_x^{j+} - U_x^{i+} = -e_n \, (U_x^{j-} - U_x^{i-})$$

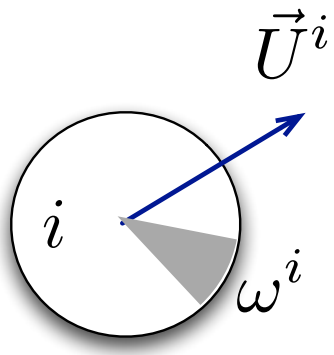
This is a kinematic constraint which works only for a binary collision (not for multiple collisions).

$$U_x^{i+} = U_x^{i-} + \frac{m^j}{m^i + m^j}(1 + e_n)(U_x^{i-} - U_x^{j-})$$

$$\Rightarrow \qquad U_x^{j+} = U_x^{j-} - \frac{m^i}{m^i + m^j}(1 + e_n)(U_x^{i-} - U_x^{j-})$$

$$P_x = \frac{m^i m^j}{m^i + m^j}(1 + e_n)(U_x^{i-} - U_x^{j-})$$

Multibody dynamics



N_p particles

Newton-Euler equations of dynamics (2D):

$$\begin{aligned} m\,\dot{\vec{U}} &= \vec{F} + \vec{F}_{ext} \\ I\,\dot{\omega} &= \mathcal{M} + \mathcal{M}_{ext} \end{aligned}$$

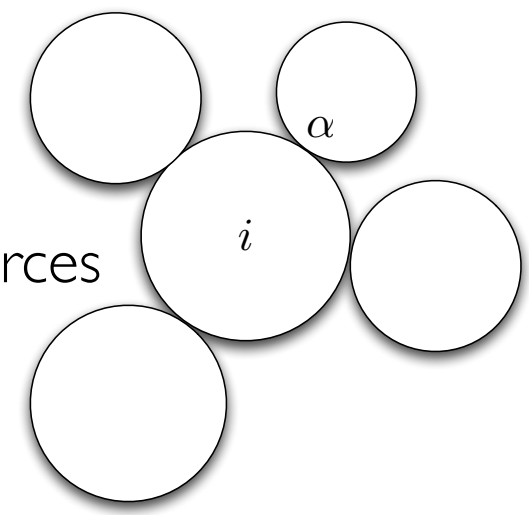
Equations of motion

$\vec{F}_{ext}$ bulk or boundary forces

$\vec{F} = \sum_\alpha \vec{f}^\alpha$ resultant of contact forces exerted by neighboring particles

$\mathcal{M}_{ext}$ moment of external forces

$\mathcal{M} = \hat{z} \cdot \sum_\alpha \vec{c}^\alpha \times \vec{f}^\alpha$ total moment of contact forces



$\vec{c}^\alpha$ contact vector

Hence, the equations of dynamics should be written as the equality of measures

$$\begin{aligned} m\ d\vec{U} &= d\vec{F}' + \vec{F}_{ext}\ dt \\ I\ d\omega &= d\mathcal{M}' + \mathcal{M}_{ext}\ dt \end{aligned}$$

Integration over the time increment yields

$$\begin{aligned} m\ (\vec{U}^+ - \vec{U}^-) &= \delta t\ \vec{F} + \delta t\ \vec{F}_{ext} \\ I\ (\omega^+ - \omega^-) &= \delta t\ \mathcal{M} + \delta t\ \mathcal{M}_{ext} \end{aligned}$$

where $\int_t^{t+\delta t} d\vec{F}' = \vec{F}\ \delta t$ $\int_t^{t+\delta t} d\mathcal{M}' = \mathcal{M}\ \delta t$

$\vec{F}$ is a coarse-grained force and its dynamic content depends on time resolution.

Matrix representation

The particles are labelled with integers: $i \in [1, N_p]$

The forces and force moments acting on the particles are arranged in a single high-dimensional column vector represented by a boldface letter. In the same way, external bulk forces applied on the particles and the particle velocity components are represented by column vectors. The particle masses and moments of inertia define a diagonal matrix.:

matrix writing

$$F = \begin{bmatrix} F_x^1 \\ F_y^1 \\ \mathcal{M}^1 \\ F_x^2 \\ F_y^2 \\ \mathcal{M}^2 \\ \vdots \\ F_x^{N_p} \\ F_y^{N_p} \\ \mathcal{M}^{N_p} \end{bmatrix} \qquad U = \begin{bmatrix} U_x^1 \\ U_y^1 \\ \omega^1 \\ U_x^2 \\ U_y^2 \\ \omega^2 \\ \vdots \\ U_x^{N_p} \\ U_y^{N_p} \\ \omega^{N_p} \end{bmatrix} \qquad M = \begin{bmatrix} m^1 & 0 & 0 & 0 & 0 & 0 \\ 0 & m^1 & 0 & 0 & 0 & 0 \\ 0 & 0 & I^1 & 0 & 0 & 0 \\ \cdots & & & & & \\ 0 & 0 & 0 & m^{N_p} & 0 & 0 \\ 0 & 0 & 0 & 0 & m^{N_p} & 0 \\ 0 & 0 & 0 & 0 & 0 & I^{N_p} \end{bmatrix}$$

The system of equations can then be written as a single matrix equation:

$$M(U^+ - U^-) = \delta t(F + F_{ext})$$

$$F, U^-, U^+, F_{ext} \in \mathbb{R}^{3N_p} \qquad M \in \mathbb{R}^{3N_p} \times \mathbb{R}^{3N_p}$$

Signorini

$$\begin{cases} \delta_n > 0 & \Rightarrow & f_n = 0 \\ \delta_n = 0 & \wedge & \begin{cases} u_n > 0 & \Rightarrow & f_n = 0 \\ u_n = 0 & \Rightarrow & f_n \geq 0 \end{cases} \end{cases}$$

Coulomb

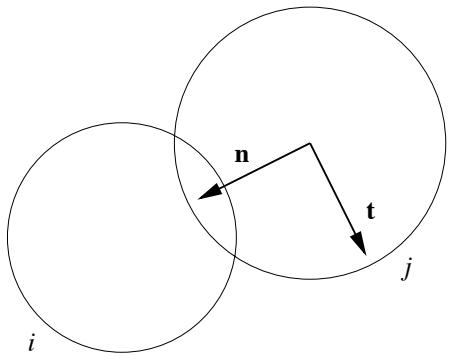
$$\begin{cases} u_t > 0 & \Rightarrow & f_t = -\mu f_n \\ u_t = 0 & \Rightarrow & -\mu f_n \leq f_t \leq \mu f_n \\ u_t < 0 & \Rightarrow & f_t = \mu f_n \end{cases}$$

Given U^- and a time resolution δt , find U^+ and (f_n, f_t) satisfying the equations of dynamics and frictional contact inequalities.

Contact velocities are expressed as a function of particle velocities :

$$u_n = \left(\mathbf{U}^i - \mathbf{U}^j\right) \cdot \mathbf{n}$$

$$u_t = \left(\mathbf{U}^i - \mathbf{U}^j\right) \cdot \mathbf{t} - \left(a_i \mathbf{\Omega}^i + a_j \mathbf{\Omega}^j\right) \times \mathbf{n}$$



The contacts are labelled with integers $\alpha \in [1, N_c]$

The normal and tangential contact velocities can be collected in a column vector $u \in \mathbb{R}^{2N_c}$

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

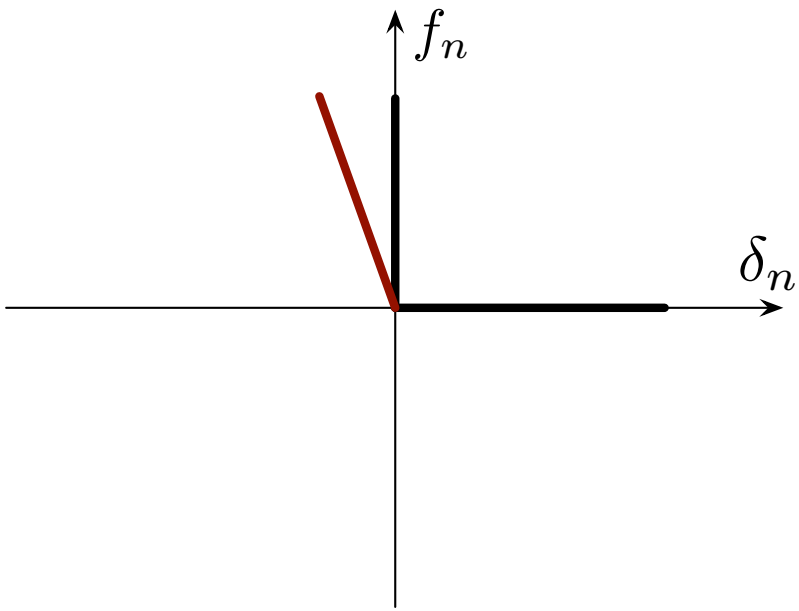
$$u = G\ U$$

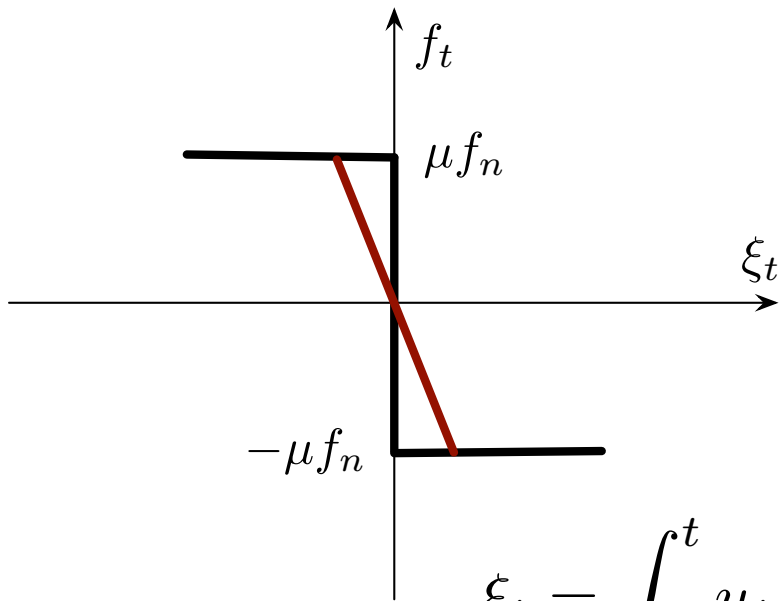
where G is a $2N_c \times 3N_p$ matrix

Molecular dynamics

Approximating the nonsmooth contact laws by regularized functions:

smoothing





$$\xi_t = \int_{t_0}^{t} u_t \, dt$$

force laws

$\Rightarrow$ force laws $\quad f_n = f_n(\delta_n, u_n) \qquad f_t = f_t(f_n, \xi_t, u_t)$

Linear dashpot model

Simplest force law of smooth DEM

$$f_n = k_n \xi_n + \gamma_n \dot{\xi}_n \qquad \text{with}$$

with $\quad \xi_n = -\delta_n \qquad \dot{\xi}_n = u_n$

$$\Rightarrow \qquad e_n = \exp\left\{ -\frac{\pi\gamma_n}{2m} \Big/ \sqrt{\frac{k_n}{m} - \left(\frac{\gamma_n}{2m}\right)^2} \right\}$$

binary collision

Correction

f_n can become negative when $\dot{\xi}_n < 0$

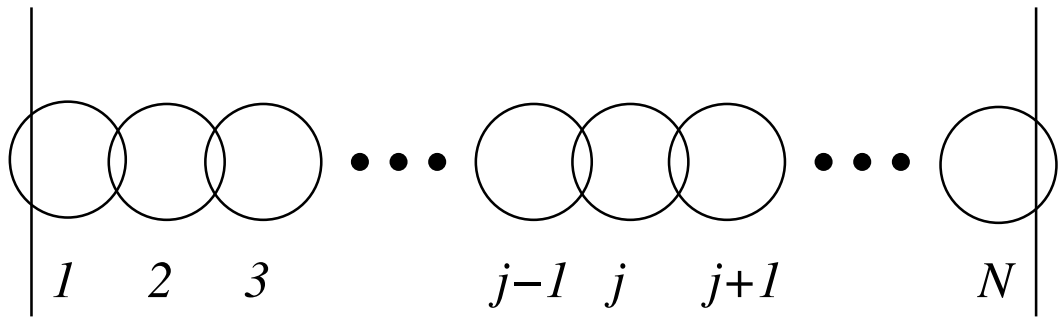
$$\Rightarrow \qquad f_n = \max\{0, k_n \xi_n + \gamma_n \dot{\xi}_n\}$$

Regularized Coulomb law

regularized friction law

$$f_t = -\text{sign}(u_t) \cdot \min\left\{|\kappa_t \xi_t|, \mu f_n\right\}$$

We consider a linear chain of grains governed by linear harmonic interactions :



$$m\frac{d^2x_j}{dt^2} = -k_n(2x_j - x_{j+1} - x_{j-1}) - \gamma_n\left(2\frac{dx_j}{dt} - \frac{dx_{j+1}}{dt} - \frac{dx_{j-1}}{dt}\right)$$

Staionary solution :

$$x_j = j\Delta x + x_0 \qquad \text{with} \quad \Delta x = L/N$$

Time-dependent solution: $x_j(t) = j\Delta x + w_j(t)$

$$w_j(t) = Ae^{s_m t} e^{i\pi m j/N}$$

$$s_m = -\mu_m \pm \sqrt{\mu_m^2 - \omega_m^2}$$

$$\omega_m = \epsilon\omega_0, \quad \mu_m = \epsilon^2\mu_0, \quad \text{with} \quad \epsilon = 2\sin\frac{\pi m}{2N}$$

$$\omega_0 = \sqrt{\frac{k}{m}}, \quad \mu_0 = \frac{\gamma}{2m}$$

For the wave $m = N$ the frequency has its highest value $2\omega_0$

To resolve the motion with sufficient precision, the time step must be smaller than $1/2\pi\omega_0$

$$\Rightarrow \quad \delta t \ll \sqrt{\frac{m}{k}}$$

time step

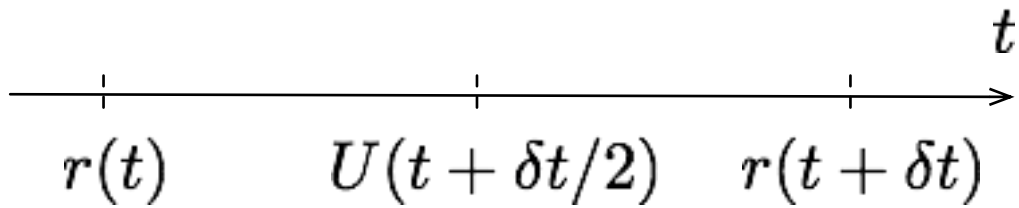
With the Herz law, the contact stiffness, and hence the characteristic frequency, increases with the load. To choose the time step, the maximum value of the normal force should be estimated.

In a granular flow, the time step must also be small enough so that the fastest grain move only a small fraction of of the their size during one time step : $\dot{\varepsilon}\delta t \ll pd/k_n$

$$\Rightarrow \qquad \delta t \ll \frac{pd}{\dot{\varepsilon} k_n}$$

Leap-frog (Verlet) scheme

The velocities are calculated at intermediate times between the grain positions.



$$U(t+\delta t/2) = U(t-\delta t/2) + a(t)\ \delta t$$

$$r(t+\delta t) = r(t) + U(t+\delta/2)\delta t$$

To calculate the forces and accelerations, it requires the positions and velocities at time t

$$U(t) = U(t-\delta t/2) + a(t-\delta t)\delta t/2$$

Gear's predictor-corrector scheme

Prediction (Taylor expansion of all degrees of freedom)

$$\vec{r}^{\,p}(t+\delta t) = \vec{r}^{\,p}(t) + \delta t\ \dot{\vec{r}}(t) + \frac{1}{2}\delta t^2\ \ddot{\vec{r}}(t) + \frac{1}{6}\delta t^3\ \dddot{\vec{r}}(t) + \dots$$

$$\dot{\vec{r}}^{\,p}(t+\delta t) = \dot{\vec{r}}^{\,p}(t) + \delta t\ \ddot{\vec{r}}(t) + \frac{1}{2}\delta t^2\ \dddot{\vec{r}}(t) + \dots$$

$$\ddot{\vec{r}}^{\,p}(t+\delta t) = \ddot{\vec{r}}^{\,p}(t) + \delta t\ \dddot{\vec{r}}(t) + \dots$$

$$\vdots$$

Force computation (for the predicted values)

$$\vec{F}^i(\vec{r}^{\,p}, \vec{U}^p) \qquad \vec{\mathcal{M}}^i(\vec{r}^{\,p}, \vec{U}^p) \quad \Rightarrow$$

$$\ddot{\vec{r}}^{\,c}(t+\delta t) \quad \ddot{\theta}^{\,c}(t+\delta t)$$

Correction

$$\Delta\ddot{\vec{r}} = \ddot{\vec{r}}^{\,c} - \ddot{\vec{r}}^{\,p}$$

$$\vec{r}^{\,c}(t+\delta t) = \vec{r}^{\,p}(t+\delta t) + c_0 \frac{1}{2}(\delta t)^2 \Delta\ddot{\vec{r}}$$

$$\dot{\vec{r}}^{\,c}(t+\delta t) = \dot{\vec{r}}^{\,p}(t+\delta t) + c_1 \frac{1}{2}(\delta t) \Delta\ddot{\vec{r}}$$

$$\ddot{\vec{r}}^{\,c}(t+\delta t) = \ddot{\vec{r}}^{\,p}(t+\delta t) + c_2 \Delta\ddot{\vec{r}}$$

$$\dddot{\vec{r}}^{\,c}(t+\delta t) = \dddot{\vec{r}}^{\,p}(t+\delta t) + c_3 \; 3(\delta t)^{-1} \Delta\ddot{\vec{r}}$$

$$\vdots$$

For an expansion of fifth order:

$$c_0 = \frac{19}{90} \quad c_1 = \frac{3}{4} \quad c_2 = 1 \quad c_3 = \frac{1}{2} \quad c_4 = \frac{1}{12}$$

Contact dynamics

Dynamics

$$M(U^+ - U^-) = \delta t(F + F_{ext})$$

Signorini

$$\begin{cases} \delta_n > 0 & \Rightarrow & f_n = 0 \\ \delta_n = 0 & \wedge & \begin{cases} u_n > 0 & \Rightarrow & f_n = 0 \\ u_n = 0 & \Rightarrow & f_n \geq 0 \end{cases} \end{cases}$$

Coulomb

$$\begin{cases} u_t > 0 & \Rightarrow & f_t = -\mu f_n \\ u_t = 0 & \Rightarrow & -\mu f_n \leq f_t \leq \mu f_n \\ u_t < 0 & \Rightarrow & f_t = \mu f_n \end{cases}$$

We need to express the equations of dynamics in contact variables.

The contacts are labelled with integers $\alpha \in [1, N_c]$

The normal and tangential contact velocities can be collected in a column vector $u \in \mathbb{R}^{2N_c}$

In the same way, the normal and tangential contact forces are represented by a vector $f \in \mathbb{R}^{2N_c}$

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

A similar linear application relates f to F.

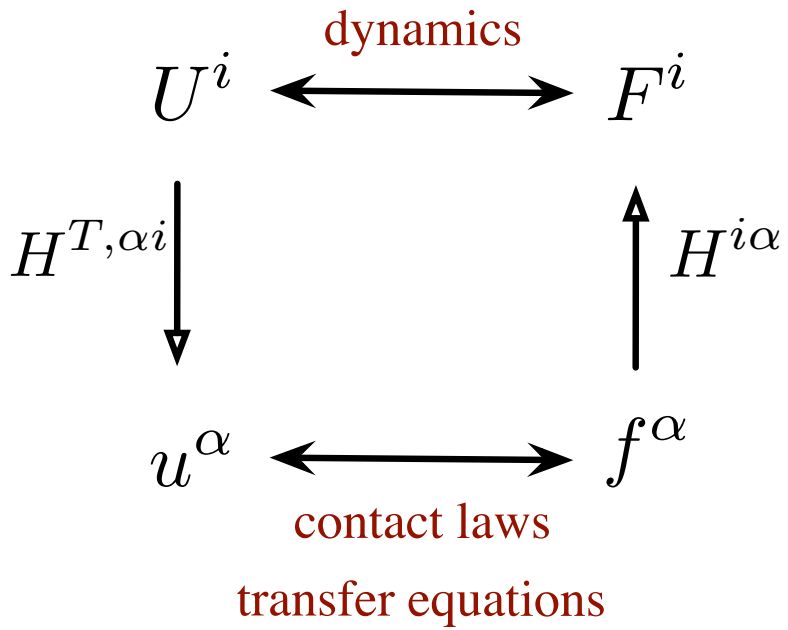
$$u = G\ U$$

$$F = H\ f$$

where

G $2N_c \times 3N_p$ matrix

H $3N_p \times 2N_c$ matrix



Equality of powers $F \cdot U = f \cdot u \quad \Rightarrow \quad H = G^T$

Contact matrix

The contact matrix is generally singular and its null space has a dimension at least equal to $2N_c - 3N_p$

Decomposition: $H^{i\alpha} = H_n^{i\alpha} + H_t^{i\alpha}$

$$u_n^\alpha = \sum_i H_n^{T,\alpha i}\ U^i$$

$$u_t^\alpha = \sum_i H_t^{T,\alpha i}\ U^i$$

$\Rightarrow$ The equations of dynamics can be transformed into two equations for each contact:

$$
\begin{aligned}
u_n^{\alpha+} - u_n^{\alpha-} &= \delta t \sum_{i,j} H_n^{T,\alpha i}\ M^{-1,ij}\ \{\sum_{\beta}(H_n^{j\beta} f_n^{\beta} + H_t^{j\beta} f_t^{\beta}) + F_{ext}^{j}\} \\
u_t^{\alpha+} - u_t^{\alpha-} &= \delta t \sum_{i,j} H_t^{T,\alpha i}\ M^{-1,ij}\ \{\sum_{\beta}(H_n^{j\beta} f_n^{\beta} + H_t^{j\beta} f_t^{\beta}) + F_{ext}^{j}\}
\end{aligned}
$$

$$
u_n = \frac{u_n^{+} + e_n\ u_n^{-}}{1+e_n} \qquad u_t = \frac{u_t^{+} + e_t\ u_t^{-}}{1+e_t}
$$

$$
\begin{aligned}
\frac{1+e_n}{\delta t}\ (u_n^{\alpha} - u_n^{\alpha-}) &= \mathcal{W}_{nn}^{\alpha\alpha} f_n^{\alpha} + \mathcal{W}_{nt}^{\alpha\alpha} f_t^{\alpha} \\
&+ \sum_{\beta(\neq\alpha)} \{\mathcal{W}_{nn}^{\alpha\beta} f_n^{\beta} + \mathcal{W}_{nt}^{\alpha\beta} f_t^{\beta}\} + \sum_{i,j} H_n^{T,\alpha i} M^{-1,ij} F_{ext}^{j} \\
\frac{1+e_t}{\delta t}\ (u_t^{\alpha} - u_t^{\alpha-}) &= \mathcal{W}_{tn}^{\alpha\alpha} f_n^{\alpha} + \mathcal{W}_{tt}^{\alpha\alpha} f_t^{\alpha} \\
&+ \sum_{\beta(\neq\alpha)} \{\mathcal{W}_{tn}^{\alpha\beta} f_n^{\beta} + \mathcal{W}_{nt}^{\alpha\beta} f_t^{\beta}\} + \sum_{i,j} H_t^{T,\alpha i} M^{-1,ij} F_{ext}^{j}
\end{aligned}
$$

where

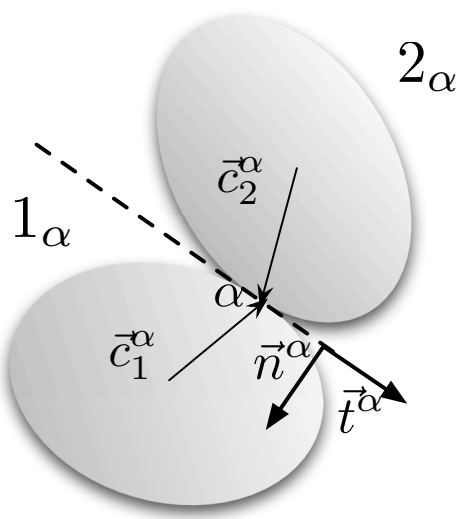
$$\mathcal{W}^{\alpha\beta}_{k_1 k_2} = \sum_{i,j} H^{T,\alpha i}_{k_1} M^{-1,ij} H^{j\beta}_{k_2}$$

inverse reduced inertia

$$\mathcal{W}^{\alpha\alpha}_{nn} = \frac{1}{m_{1_\alpha}} + \frac{1}{m_{2_\alpha}} + \frac{(c^\alpha_{1t})^2}{I_{1_\alpha}} + \frac{(c^\alpha_{2t})^2}{I_{2_\alpha}}$$

$$\mathcal{W}^{\alpha\alpha}_{tt} = \frac{1}{m_{1_\alpha}} + \frac{1}{m_{2_\alpha}} + \frac{(c^\alpha_{1n})^2}{I_{1_\alpha}} + \frac{(c^\alpha_{2n})^2}{I_{2_\alpha}}$$

$$\mathcal{W}^{\alpha\alpha}_{nt} = \mathcal{W}^{\alpha\alpha}_{tn} = \frac{c^\alpha_{1n} c^\alpha_{1t}}{I_{1_\alpha}} + \frac{c^\alpha_{2n} c^\alpha_{2t}}{I_{2_\alpha}}$$



with

$$c^\alpha_{in} = \vec{c}^\alpha_i \cdot \vec{n}^\alpha$$

$$c^\alpha_{it} = \vec{c}^\alpha_i \cdot \vec{t}^\alpha$$

Alternative representation :

$$\begin{aligned} \mathcal{W}_{nn}^{\alpha\alpha} f_n^\alpha + \mathcal{W}_{nt}^{\alpha\alpha} f_t^\alpha &= (1+e_n)\,\frac{1}{\delta t} u_n^\alpha + a_n^\alpha \\ \mathcal{W}_{tt}^{\alpha\alpha} f_t^\alpha + \mathcal{W}_{tn}^{\alpha\alpha} f_n^\alpha &= (1+e_t)\,\frac{1}{\delta t} u_t^\alpha + a_t^\alpha \end{aligned}$$

transfer equations

with

$$\begin{aligned} a_n^\alpha &= b_n^\alpha - (1+e_n)\frac{1}{\delta t}\, u_n^{\alpha-} + \left(\frac{\vec{F}_{ext}^{2_\alpha}}{m_{2_\alpha}} - \frac{\vec{F}_{ext}^{1_\alpha}}{m_{1_\alpha}} \right) \cdot \vec{n}^\alpha \\ a_t^\alpha &= b_t^\alpha - (1+e_t)\frac{1}{\delta t}\, u_t^{\alpha-} + \left(\frac{\vec{F}_{ext}^{2_\alpha}}{m_{2_\alpha}} - \frac{\vec{F}_{ext}^{1_\alpha}}{m_{1_\alpha}} \right) \cdot \vec{t}^\alpha \end{aligned}$$

offsets

and

$$\begin{aligned} b_n^\alpha &= \frac{1}{m_{2_\alpha}} \sum_{\beta(\neq\alpha)} \vec{f}_{2_\alpha}^{\beta} \cdot \vec{n}^\alpha - \frac{1}{m_{1_\alpha}} \sum_{\beta(\neq\alpha)} \vec{f}_{1_\alpha}^{\beta} \cdot \vec{n}^\alpha \\ b_t^\alpha &= \frac{1}{m_{2_\alpha}} \sum_{\beta(\neq\alpha)} \vec{f}_{2_\alpha}^{\beta} \cdot \vec{t}^\alpha - \frac{1}{m_{1_\alpha}} \sum_{\beta(\neq\alpha)} \vec{f}_{1_\alpha}^{\beta} \cdot \vec{t}^\alpha \end{aligned}$$

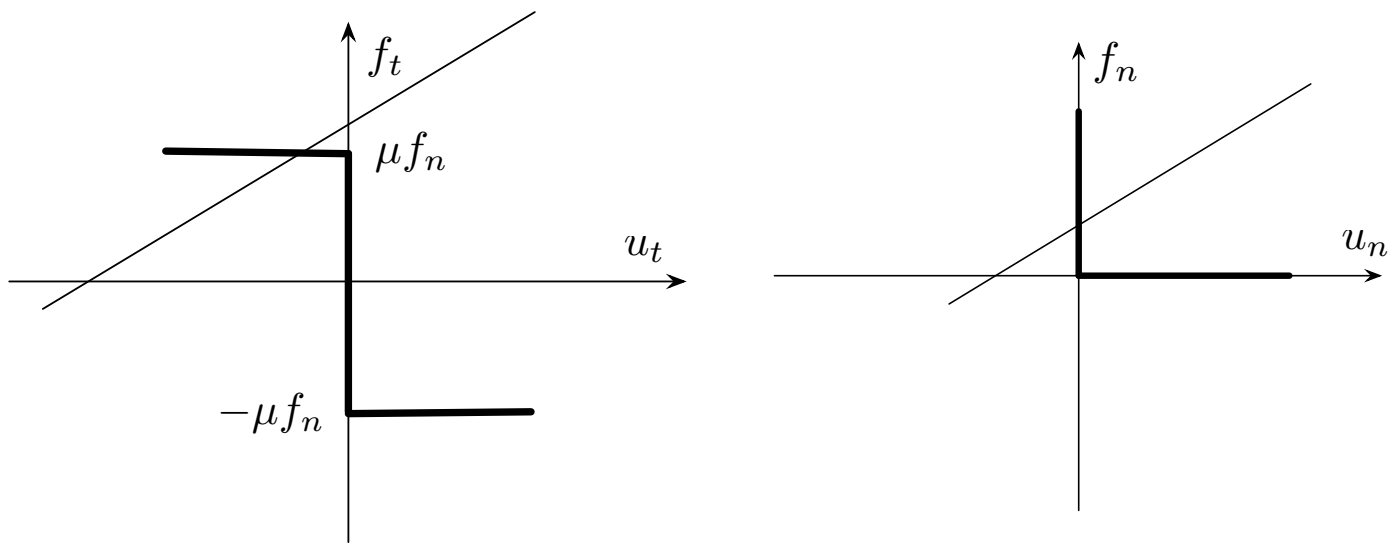
coupling terms with other particles

Iterative resolution

In order to solve the system of transfer equations (in 2D) with the corresponding complementarity relations, we proceed by an iterative method which converges to the solution simultaneously for all contact forces and velocities.

Single contact problem

Determine $f_n^\alpha, f_t^\alpha, u_n^\alpha, u_t^\alpha$ at a single contact given the values of the offsets a_n^α and a_t^α at the same contact: local Singnorini-Coulomb (SC) problem.



The two transfer equations are generally coupled and thus the two intersections can not be established separately.

We consider the inersection of the transfer equations with the force axis by setting $u_n = u_t = 0$

$$
\begin{aligned}
g_n^\alpha &= \frac{\mathcal{W}_{tt}^{\alpha\alpha} a_n^\alpha - \mathcal{W}_{nt}^{\alpha\alpha} a_t^\alpha}{\mathcal{W}_{nn}^{\alpha\alpha}\mathcal{W}_{tt}^{\alpha\alpha} - (\mathcal{W}_{nt}^{\alpha\alpha})^2} \\
g_t^\alpha &= \frac{\mathcal{W}_{nn}^{\alpha\alpha} a_n^\alpha - \mathcal{W}_{tn}^{\alpha\alpha} a_t^\alpha}{\mathcal{W}_{tt}^{\alpha\alpha}\mathcal{W}_{nn}^{\alpha\alpha} - (\mathcal{W}_{tn}^{\alpha\alpha})^2}
\end{aligned}
$$

$g_n^\alpha < 0 \Rightarrow \quad f_n^\alpha = f_t^\alpha = 0$ breaking contact

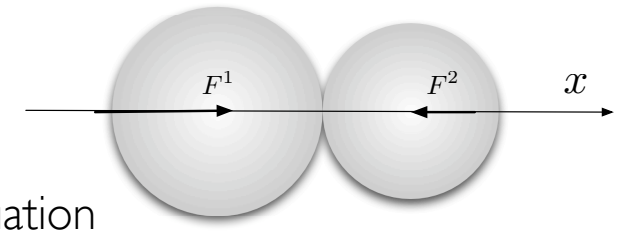
$g_t^\alpha > \mu f_n^\alpha \Rightarrow f_t^\alpha = \mu f_n^\alpha$ sliding contact

$g_n^\alpha \geq 0 \Rightarrow \quad f_n^\alpha = g_n^\alpha \qquad g_t^\alpha < -\mu f_n^\alpha \Rightarrow f_t^\alpha = -\mu f_n^\alpha$

$-\mu f_n^\alpha < g_t^\alpha < \mu f_n^\alpha \Rightarrow f_t^\alpha = g_t^\alpha$ rolling contact

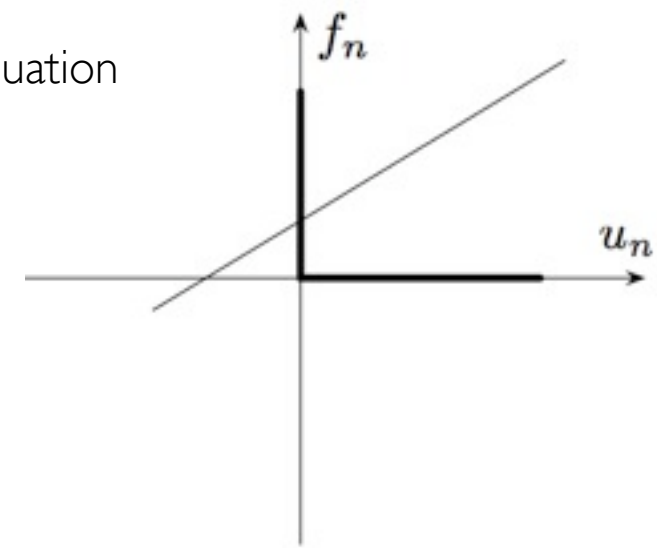
Resolved and unresolved forces

Example of head-on collision under the action of two parallel forces



$$\mathcal{W}_{nn} f_n = (1 + e_n)\frac{1}{\delta t} u_n + a_n$$ transfer equation

$$a_n = -(1 + e_n)\frac{1}{\delta t}\, u_n^- + \left(\frac{F^1}{m_1} + \frac{F^2}{m_2}\right)$$ offset equation



The collision implies $u_n = 0$

$$\Rightarrow \quad u_n^+ = -e_n u_n^-$$

$$\Rightarrow \quad f_n = a_n = -\frac{1}{\delta t}\frac{m_1 m_2}{m_1 + m_2}(1 + e_n)\, u_n^- + \left(\frac{m_2 F^1 + m_1 F^2}{m_1 + m_2}\right)$$

unresolved force — resolved force

In the CD method, the impulsive force decreases with time step.

$$u_n^- = 0 \quad \Rightarrow \quad u_n^+ = 0 \qquad f_n = \frac{m_2 F^1 + m_1 F^2}{m_1 + m_2}$$

$$U^{1+} = U^{1-} + \delta t \frac{F^1 - f_n}{m_1}$$

$$U^{2+} = U^{2-} + \delta t \frac{-F^2 + f_n}{m_2}$$

$$U^{1-} = U^{2-} = 0$$

Particles initially at rest

$$\Rightarrow \quad U^{1+} = U^{2+} = \frac{F^1 - F^2}{m_1 + m_2}$$

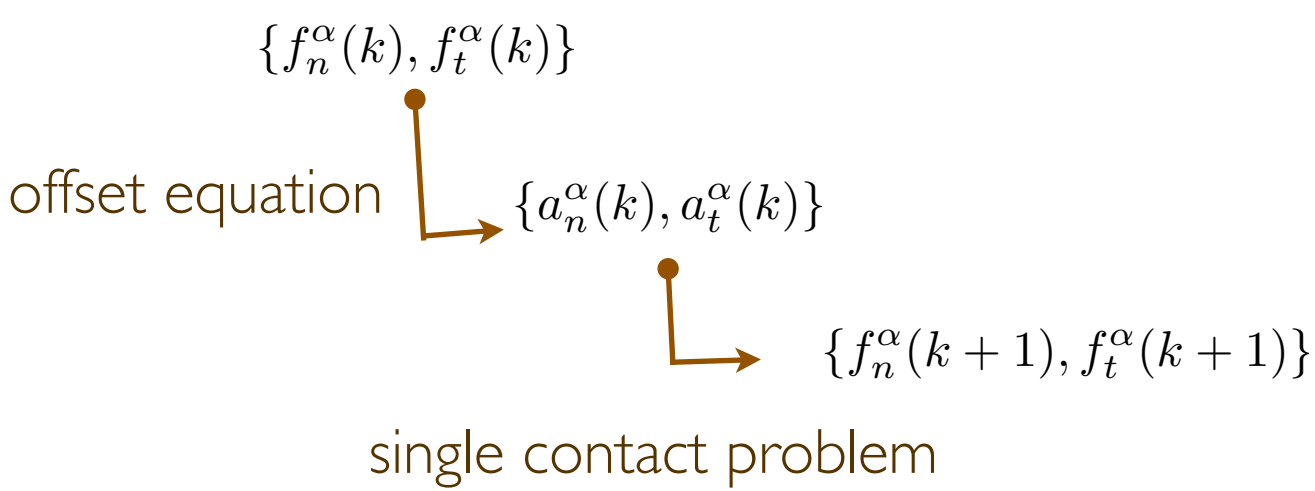
Center-of-mass velocity

Multicontact problem

The solution for each contact depends on all other contacts of the system and it must be determined simultaneously for all contacts. This is the global Singnorini-Coulomb (SC) problem.

We search the solution as the limit of a sequence

$$\{f_n^\alpha(k), f_t^\alpha(k), u_n^\alpha(k), u_t^\alpha(k)\} \qquad \alpha \in [1, N_c]$$



The set $\{f_n^\alpha(k), f_t^\alpha(k)\}$ evolves with k by successive corrections and it converges to a solution satisfying the transfer equations and complementarity relations at all potential contacts of the system.

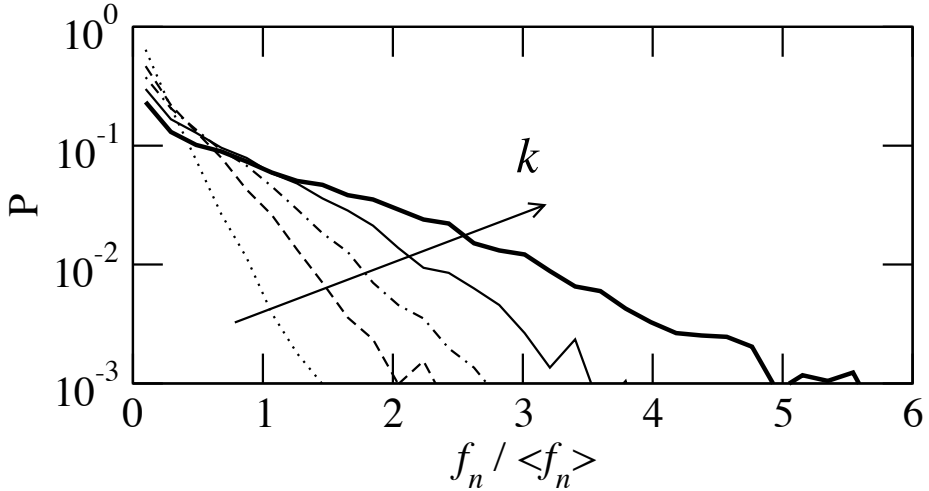
The iteration is stopped when a precision criterion is satisfied:

$$\frac{\mid f^{\alpha}(k+1) - f^{\alpha}(k) \mid}{f^{\alpha}(k+1)} < \varepsilon_f \quad \forall \alpha$$

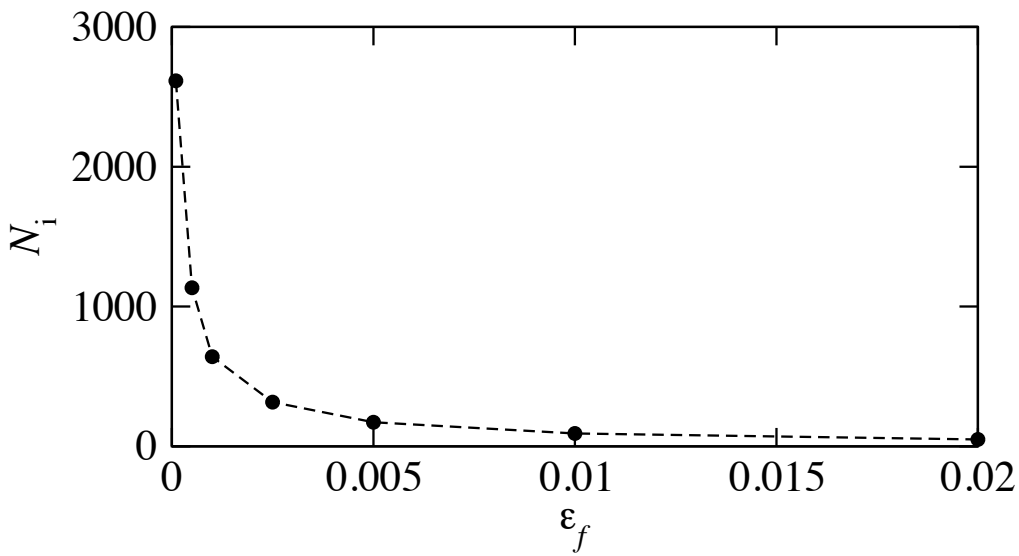
From the converged contact forces, the particle velocities can be computed by means of the equations of dynamics

This is a robust procedure. Moreover, the information is treated locally and no large matrices are manipulated during iterations.

The number of required iterations for convergence depends on the precision, the initialization (first guess) of the forces and the propagation of the information (ordering).



Evolution of the probability density of normal forces with iterations. The forces are normalized by the mean force at the converged state.



The number of iterations (for initially zero forces) as a function of convergence criterion.

Time-stepping

The global SC problem may well occur as an event at particular instances of a granular flow. The iterative resolution method can then be applied to calculate the contact forces and particle velocities at those instances. But in dense multicontact granular media the events cannot be predicted.

In the CD method, the global SC problem is embedded in a time-stepping scheme. This scheme is based on two features of the nonsmooth framework:

1) The multicontact SC problem is formulated at the velocity level for both dynamics and contact laws, and the position-Signorini condition is accounted for by involving only the eligible contacts, determined geometrically, in the SC problem. Hence, in a time-stepping scheme, the contact network should be defined explicitly from particle positions and it will no more evolve during a time step.

2) The right-limit velocities are calculated such that the complementarity relations will not be violated by the subsequent motion of the particles. This feature is named viability lemma by Moreau. It is ensured by the following condition as a consequence of the velocity-Signorini condition:

$$\delta_n \leq 0 \quad \Rightarrow \quad u_n^+ \geq 0$$

Hence, the numerical treatment is implicit and the right-limit velocities should be used to increment particle positions.

A typical scheme

$[t, t+\delta t]$ time step

$\{\vec{r}^i(t), \theta^i(t)\}$ $\{\vec{U}^i(t), \omega^i(t)\}$ Positions and velocities at the beginning of the time step

The left-limit velocities are the velocities at the beginning of the time step:

$$\vec{U}^{i-} = \vec{U}^i(t)$$
$$\omega^{i-} = \omega^i(t)$$

1) The particles are moved to the half-step configuration:

$$\vec{r}^i_m \equiv \vec{r}^i(t) + \frac{\delta t}{2}\ \vec{U}^i(t)$$

2) The contact network is set up from this configuration

$$\{\alpha, \vec{n}^\alpha, \vec{t}^\alpha\}$$

3) The global SC problem is solved iteratively for this contact network and the right-limit particle velocities are calculated. These are the right-limit velocities.

$$\vec{U}^i(t+\delta t) = \vec{U}^{i+}$$
$$\omega^i(t+\delta t) = \omega^{i+}$$

4) The positions are updated for the remaining half-step:

$$\begin{aligned}
\vec{r}^{\,i}(t+\delta t) &= \vec{r}^{\,i}_m + \frac{\delta t}{2}\,\vec{U}^i(t+\delta t) \\
\theta^i(t+\delta t) &= \theta^i_m + \frac{\delta t}{2}\,\omega^i(t+\delta t)
\end{aligned}$$

This scheme is unconditionally stable due to its implicit nature. Hence, no damping parameters at any level are needed. For this reason, the time step can be large.

The time step controls only the position updates. The precision on the velocities and forces is controlled by the convergence criterion. The time step should rather be considered as a coarse-graining parameter for nonsmooth dynamics. It should be reduced if the impulse dynamics at small time scales is of interest.

Extensions

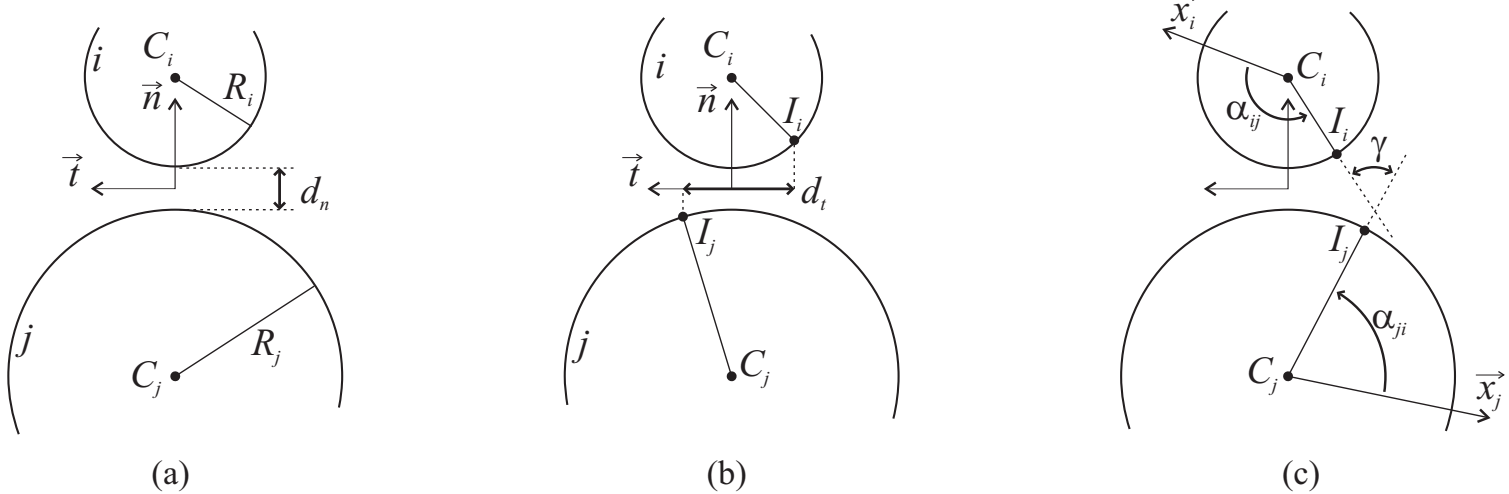
Rolling resistance: Complementarity relations are introduced between a torque and a contact spin variable.

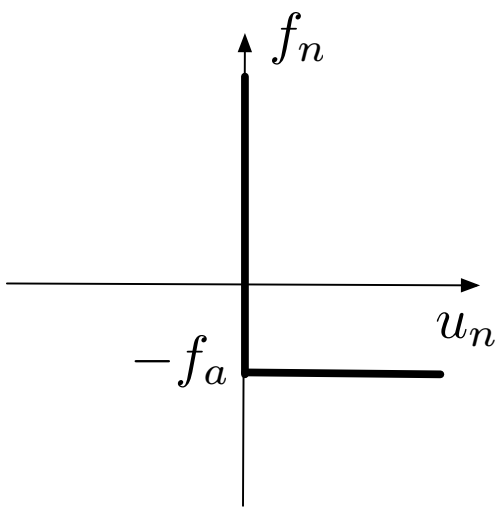
Adhesion: The complementarity relations are shifted.

Particle deformability: Elastic interactions are introduced by associating strain variables to the particles rather than to the contacts. The strains can be defined either from rigid-body degrees of freedom or associated with new internal degrees of freedom.

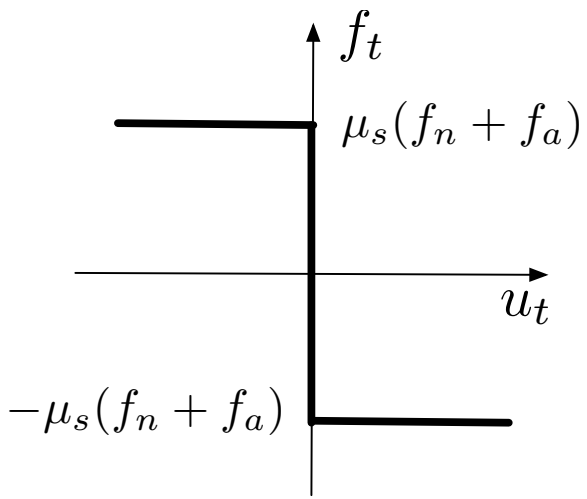
Particle shape: It is a generic feature of the CD method that, in contrast to force laws, the nature of the contact complementarity relations does not depend on the particle shape. Hence, the solver which handles the resolution of the global SC problem is independent of the particle shape. The potential face-face or face-edge contacts are represented by three or two points which are treated as independent point contacts by the solver.

Cohesion = Freezing of relative degrees of freedom between particles

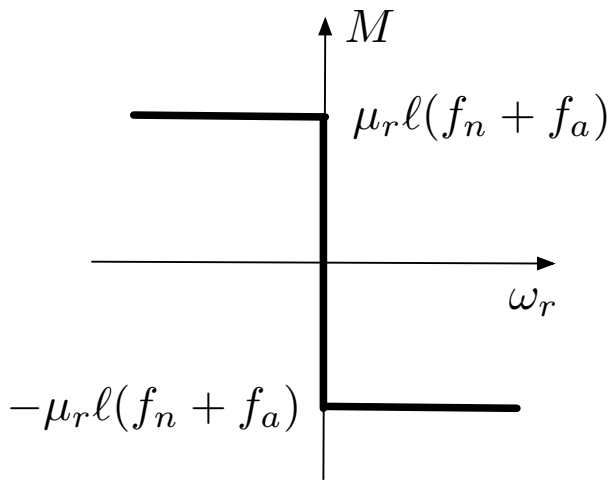




Signorini



Sliding friction law



Rolling friction law

$$\omega_r = \omega_1 - \omega 2$$

ℓ branch-vector length

Conclusions

Advanced DEM simulations based on the particle-scale dynamics provide new insights into the physical mechanisms that underly the rheology of granular materials.

Some complex features are generic and depend only quantitatively on the composition and nature of interactions.

But the influence of composition and interactions can be evaluated through the statistical descriptors of the microstructure and force anisotropy.

DEM can be used with allied methods (LEM, LBM) for the simulation of immersed and unsaturated granular materials.