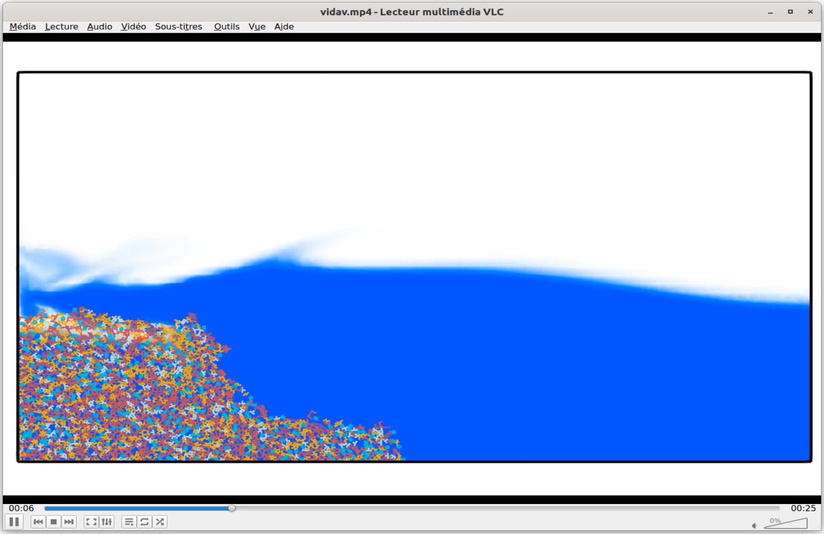
Lecture 7: fifty shapes of grains



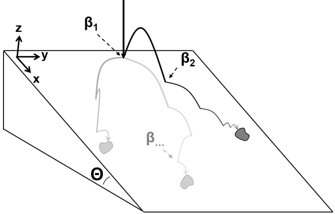
Modelling grain shapes

Asymmetric bodies in NSCD

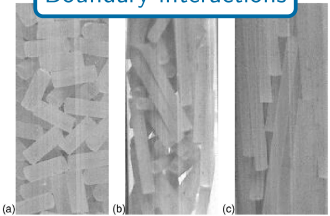
Avalanches of elongated grains

Grain shape is an important characteristic

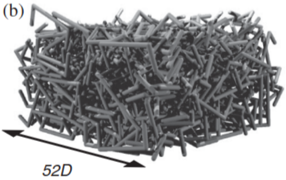
Rolling resistance



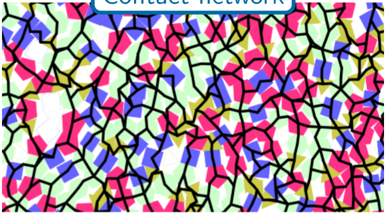
Boundary interactions



Entanglement

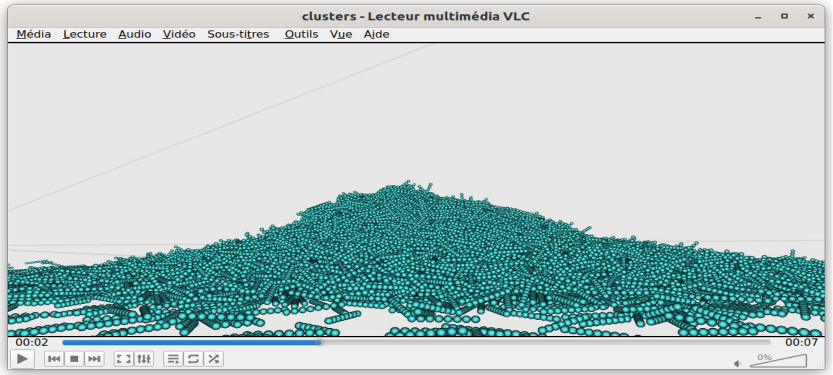


Contact network



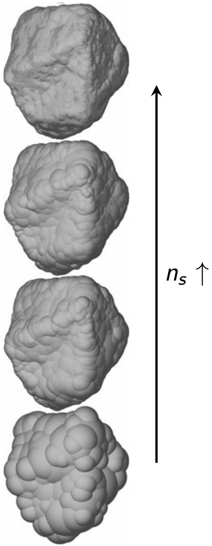
Williams & Furbish (2021), Binaree et al (2019), Gravish et al (2012), Lumay & Vandewalle (2004).

Sphere clusters



- Computationally convenient
- Fluid coupling straightforward
- Rough grain surface
- Less dense material

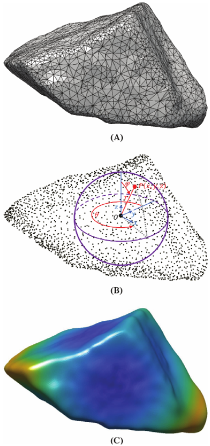
Overlapping spheres



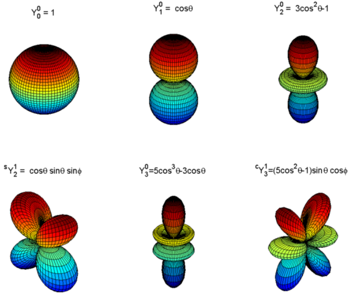
- The shape rendering is more accurate
- Contact detection is similar to spheres
- The fitting of filling parameters is more demanding
- Inertia and mass are not straightforward
- Special care is needed when computing the porosity for fluid coupling

Ferellec, J. F., McDowell, G. R. (2010). A method to model realistic particle shape and inertia in DEM. Granular Matter, 12, 459-467.

Spherical harmonics



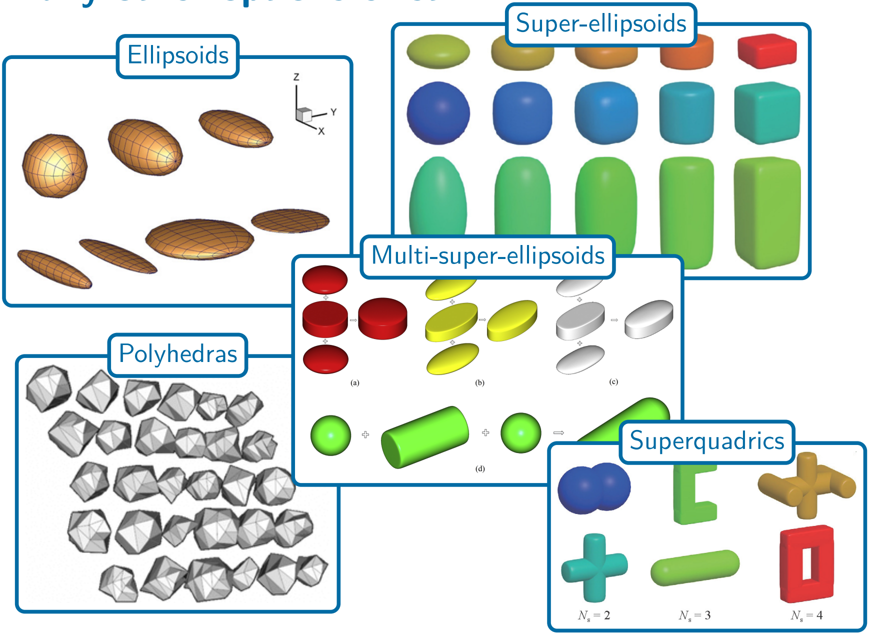
$$r(\theta,\phi) = \sum_{n=0}^{N} \sum_{m=-n}^{n} a_n^m Y_n^m(\theta,\phi)$$



- Precise for any shape
- Possible to reproduce statistically identical sets
- Many parameters a_n^m
- Contacts are difficult to detect and solve

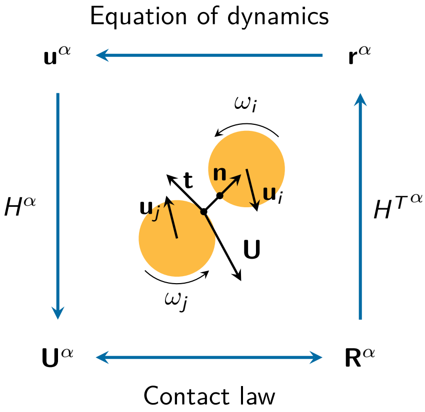
Wang, Xiang, et al. "A spherical-harmonic-based approach to discrete element modeling of 3D irregular particles." Int. Jour. for Num. Meth. in Eng. 122.20 (2021): 5626-5655.

Many other options exist



Yan et al (2010), Wang et al (2020), Liu & Zhao (2020), Nader et al (2017).

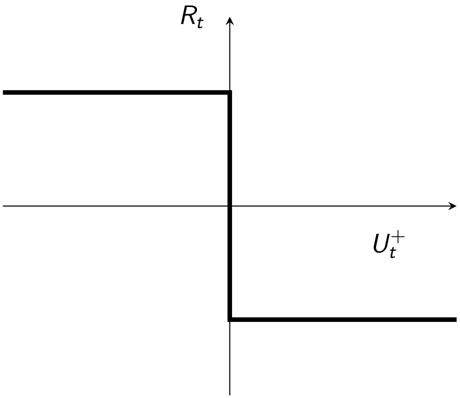
From global to local



$$\begin{pmatrix} U_n \\ U_t \end{pmatrix}^\alpha = H^\alpha \cdot \begin{pmatrix} \mathbf{u}_i \\ \omega_i \\ \mathbf{u}_j \\ \omega_j \end{pmatrix}$$

$$\mathbf{u}^\alpha = \begin{pmatrix} \mathbf{u}_i \\ \omega_i \\ \mathbf{u}_j \\ \omega_j \end{pmatrix} = {H^T}^\alpha \cdot \begin{pmatrix} U_n \\ U_t \end{pmatrix}$$

The frictional contact law



- Velocity Signorini condition:

  $U_n^+ + eU_n^- \geq 0,\ R_n \geq 0,$

  $R_n(U_n^+ + eU_n^-) = 0$

- Coulomb law:

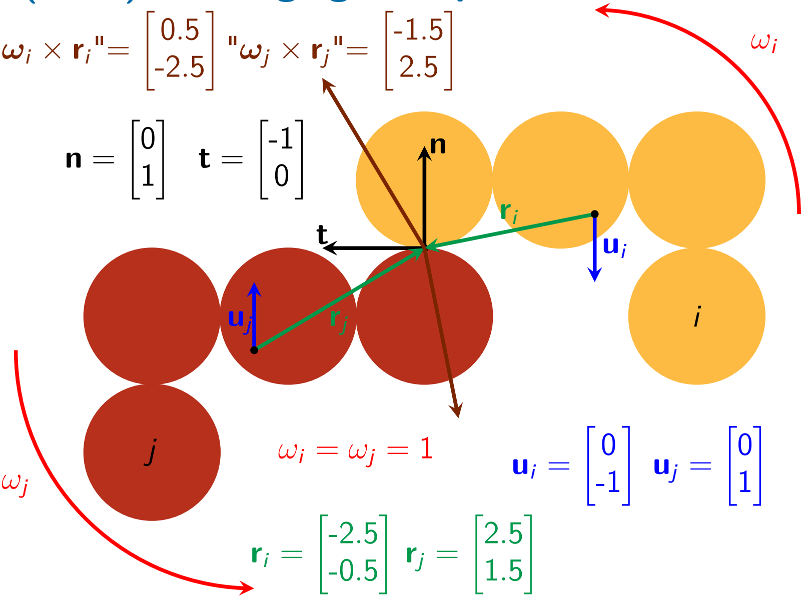
  $|\mathbf{R}_t| \leq \mu R_n,$

  $|\mathbf{U}_t^+| \neq 0 \implies \mathbf{R}_t = -\mu R_n \frac{\mathbf{U}_t^+}{|\mathbf{U}_t^+|}$

A (more) challenging example

$$"\boldsymbol{\omega}_i \times \mathbf{r}_i" = \begin{bmatrix} 0.5 \\ -2.5 \end{bmatrix} \quad "\boldsymbol{\omega}_j \times \mathbf{r}_j" = \begin{bmatrix} -1.5 \\ 2.5 \end{bmatrix}$$

$$\mathbf{n} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \mathbf{t} = \begin{bmatrix} -1 \\ 0 \end{bmatrix}$$

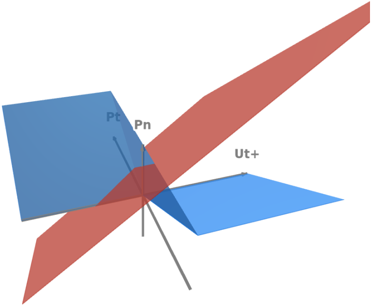


$$\omega_i = \omega_j = 1$$

$$\mathbf{u}_i = \begin{bmatrix} 0 \\ -1 \end{bmatrix} \quad \mathbf{u}_j = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\mathbf{r}_i = \begin{bmatrix} -2.5 \\ -0.5 \end{bmatrix} \quad \mathbf{r}_j = \begin{bmatrix} 2.5 \\ 1.5 \end{bmatrix}$$

Solving the general Signorini-Coulomb problem in 2D



$$P_t = (U_t^+ - U_t^- - W_{tn}P_n)/W_{tt}$$

$$U_t^+ \neq 0 \implies P_t = \mu P_n U_t^+/|U_t^+|$$

$$|P_t| \leq \mu P_n$$

If $P_t^{\text{stick}} + \mu P_n^{\text{stick}} < 0$:

$$P_t = -\mu P_n, \;\; P_n = \frac{-U_n^-}{W_{nn} - \mu W_{nt}}$$

If $P_t^{\text{stick}} - \mu P_n^{\text{stick}} > 0$:

$$P_t = \mu P_n, \;\; P_n = \frac{-U_n^-}{W_{nn} + \mu W_{nt}}$$

Else :

$$\mathbf{P} = \mathbf{P}^{\text{stick}}$$

! $-1 < -\mu W_{nt}/W_{nn} < 1$ **!**

What about the 3D problem?

If ${P_t^{\text{stick}}}^2 + {P_s^{\text{stick}}}^2 \leq \left(\mu P_n^{\text{stick}}\right)^2$:

$\boldsymbol{P} = \boldsymbol{P}^{\text{stick}}$

Else:

$$\begin{cases} W_{nn} P_n + W_{nt} P_t + W_{ns} P_s + U_n^+ - U_n^- = 0, \\ W_{nt} P_n + W_{tt} P_t + W_{ts} P_s + U_t^+ - U_t^- = 0, \\ W_{ns} P_n + W_{ts} P_t + W_{ss} P_s + U_s^+ - U_s^- = 0, \\ -\mu^2 {P_n}^2 + {P_t}^2 + {P_s}^2 = 0, \\ - U_s^+ P_t + U_t^+ P_s = 0. \end{cases}$$

- Newton-Raphson scheme
  $\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{J}^{-1}(\mathbf{x}_k)\mathbf{f}(\mathbf{x}_k)$ with $\mathbf{x} = [P_n, P_t, P_s, U_t^+, U_s^+]$
- Can we make it easier?

Geometric interpretation

- Using the linear equations to reduce the problem:
  $\mathbf{x} = [P_t, P_s] = [x, y]$

$$-\mu^2 P_n^2 + P_t^2 + P_s^2 = 0$$

↓

$$\begin{aligned}
0 = & x^2 \left[w_{nt}^2 - \left(\frac{w_{nn}}{\mu} \right)^2 \right] \\
& + xy \, [2 w_{nt} w_{ns}] \\
& + y^2 \left[w_{ns}^2 - \left(\frac{w_{nn}}{\mu} \right)^2 \right] \\
& + x \, [2 w_{nt} (U_n^+ - U_n^-)] \\
& + y \, [2 w_{ns} (U_n^+ - U_n^-)] \\
& + (U_n^+ - U_n^-)^2
\end{aligned}$$

Ellipse if $-w_{nn} < -\mu \sqrt{w_{nt}^2 + w_{ns}^2} < w_{nn}$

$$-P_s U_t^+ + P_t U_s^+ = 0$$

↓

$$\begin{aligned}
0 = & x^2 \left[w_{nt} w_{ns} - w_{nn} w_{ts} \right] \\
& - y^2 \left[w_{nt} w_{ns} - w_{nn} w_{ts} \right] \\
& + xy \left[w_{ns}^2 - w_{ss} w_{nn} - w_{nt}^2 + w_{tt} w_{nn} \right] \\
& + x \left[w_{nn} U_s^- + w_{ns} \left(U_n^+ - U_n^- \right) \right] \\
& - y \left[w_{nn} U_t^- + w_{nt} \left(U_n^+ - U_n^- \right) \right]
\end{aligned}$$

Hyperbola

- Newton-Raphson for a 2×2 system

Time discretisation

Global frame

$$\int_{t_i}^{t_{i+1}} M d\mathbf{u} = \int_{t_i}^{t_{i+1}} \mathbf{f} dt + \int_{t_i}^{t_{i+1}} \mathbf{r} d\nu$$

$$\int_{t_i}^{t_{i+1}} d\mathbf{x} = \int_{t_i}^{t_{i+1}} \mathbf{u} dt$$

With implicit Euler:

$$\mathbf{u}^{i+1} = \mathbf{u}^i + \Delta t \mathbf{M}^{-1}\left(\mathbf{f}^i + \frac{\mathbf{p}^{i+1}}{\Delta t}\right)$$

$$\mathbf{x}^{i+1} = \mathbf{x}^i + \Delta t \mathbf{u}^{i+1}$$

Local frame

Quasi-Inelastic Signorini shock law

$$\frac{\max(\mathrm{d}^i, 0)}{\Delta t} + U_n^{i+1} \geq 0,$$

$$P_n^{i+1} \geq 0,$$

$$\left(\frac{\max(\mathrm{d}^i, 0)}{\Delta t} + U_n^{i+1}\right) P_n^{i+1} = 0$$

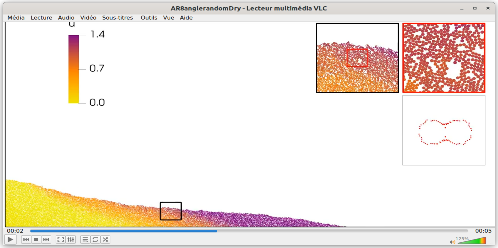
Coulomb friction law

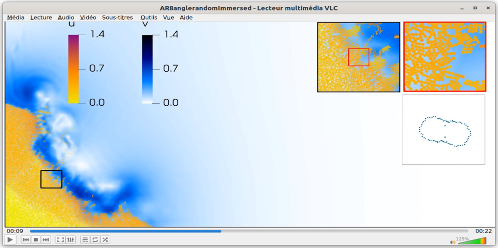
$$|\mathbf{P}_t^{i+1}| \leq \mu P_n^{i+1},$$

$$|\mathbf{U}_t^{i+1}| \neq 0 \implies \mathbf{P}_t^{i+1} = -\mu P_n^{i+1} \frac{\mathbf{U}_t^{i+1}}{|\mathbf{U}_t^{i+1}|}$$

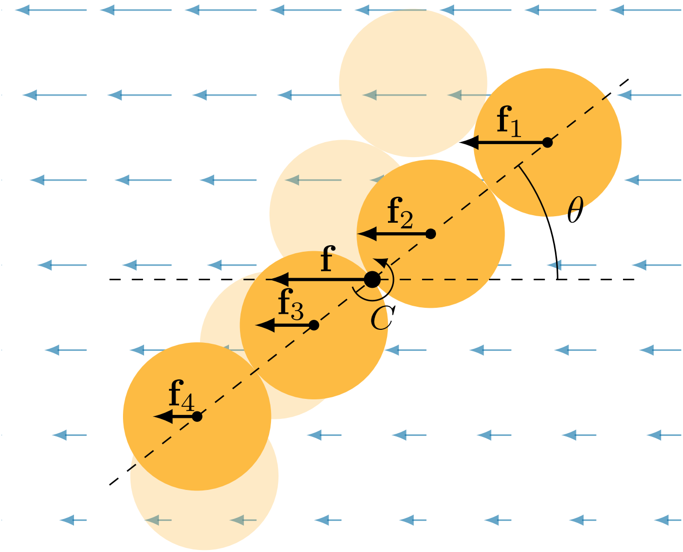
! Local frame recomputed **!**

Avalanches of elongated grains

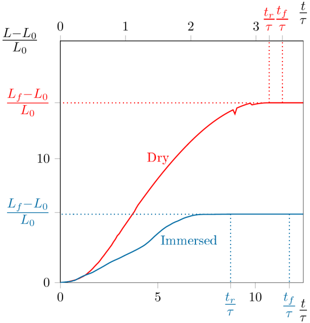


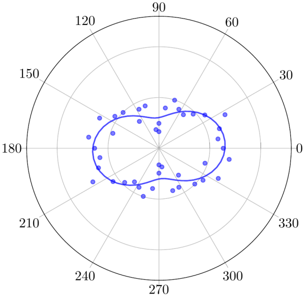


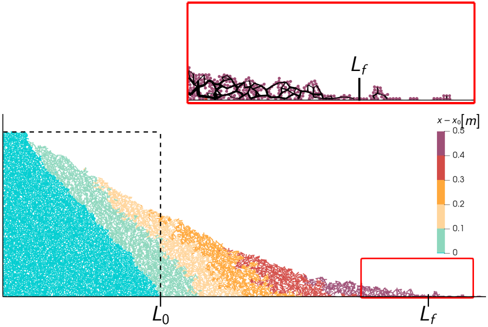
Modelling immersed elongated grains



What do we want to measure?

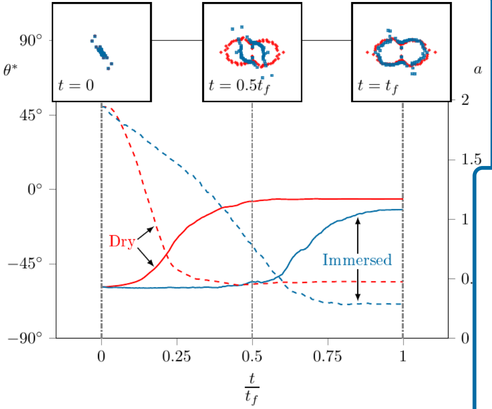


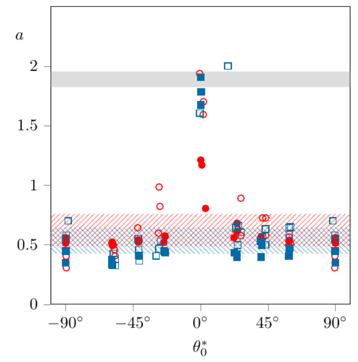




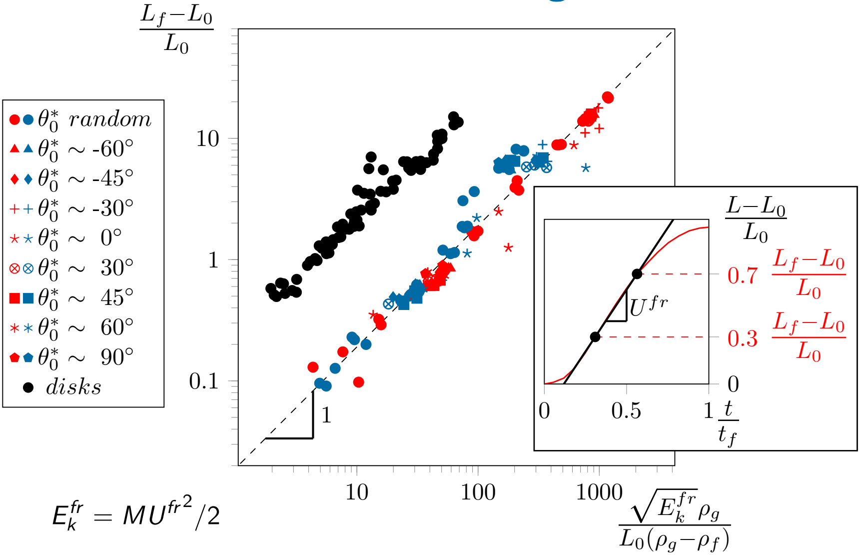
$$P(\theta) = \frac{1}{2\pi}(1 + a\cos(2(\theta - \theta^*)))$$

The orientation changes towards a universal configuration





The runout is reduced because of the orientation change



$$E_k^{fr} = M{U^{fr}}^2/2$$

Take-home messages

- Grain shape is an important parameter
- Many approaches exist to represent it
- Arbitrary shapes make the contact problem much more difficult
- The reorganisation of the microstructure of the column reduces its runout