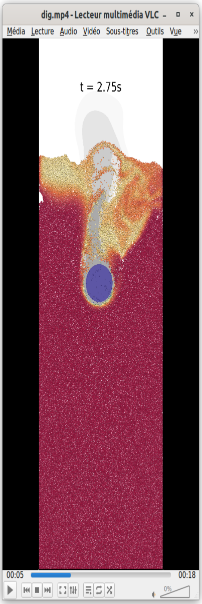
Lecture 10: Welcome to the Multiphase



Main approaches

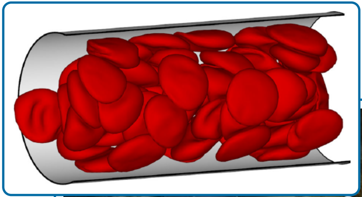
Interaction force

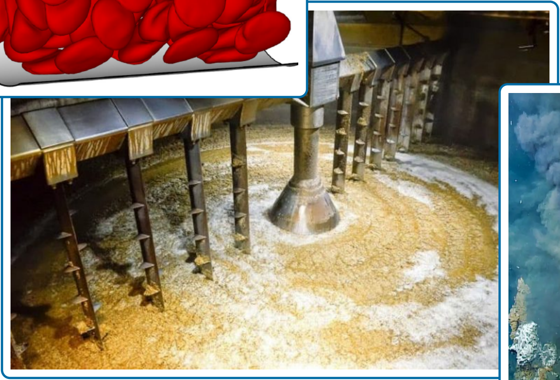
Time coupling

Heat transfer

Animation credit: Michel Henry

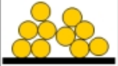
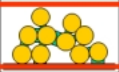
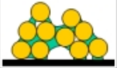
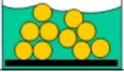
Immersed granular materials are common





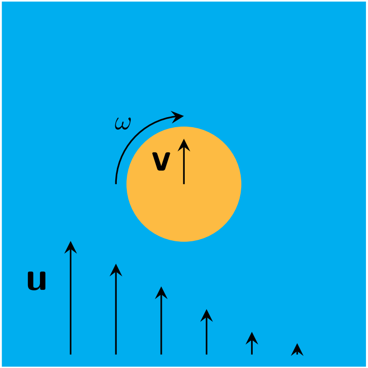
- A granular material is immersed when the ambient fluid (liquid or gas) influences its behaviour
- The Stokes number $St = \rho_g \dot{\gamma} d^2 / \eta$ and density ratio $r = \sqrt{\rho_g / \rho}$ are good indicators

The fluid influences the grains...

SATURATION DEGREE [%]	SATURATION REGIME		MEAN FORCES
0 %	Dry		Gravity, contact
0% - 5%	Pendular		Gravity, contact, capillary
5% - 35%	Funicular		Gravity, contact, capillary
35%-90%	Capillary		Gravity, contact, capillary, [drag]
90%-100%	Saturated		Gravity, contact, [drag]

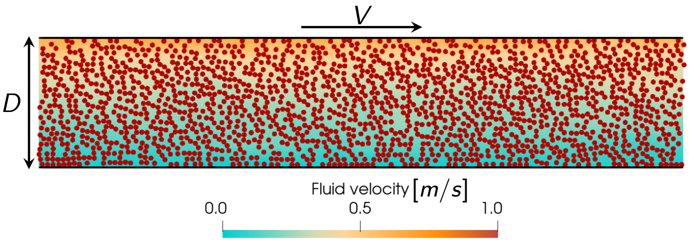
- Cohesion can be handled with a proper contact force model
- The drag force (and not only) requires a resolution of the fluid phase

The fluid influences the grains...



- Drag: $F = \frac{1}{2}\rho C_d A|\mathbf{u}-\mathbf{v}|(\mathbf{u}-\mathbf{v})$
- Pressure Gradient: $F = -V\nabla p$
- Virtual Mass: $F = \frac{\rho V}{2}(\dot{\mathbf{u}}-\dot{\mathbf{v}})$
- Basset: $F = \frac{3}{2}D^2\sqrt{\pi\rho\eta}\int_0^t \frac{\dot{\mathbf{u}}-\dot{\mathbf{v}}}{\sqrt{t-t'}dt'}$
- Saffman:
  $F = 1.61\eta D^2\sqrt{\frac{\eta\rho}{|\nabla\times\mathbf{u}|}}(\mathbf{u}-\mathbf{v}\times(\nabla\times\mathbf{u}))$
- Magnus: $F = \frac{\pi}{8}D^3\rho\omega(\mathbf{u}-\mathbf{v})$

… and the grains influence the fluid!



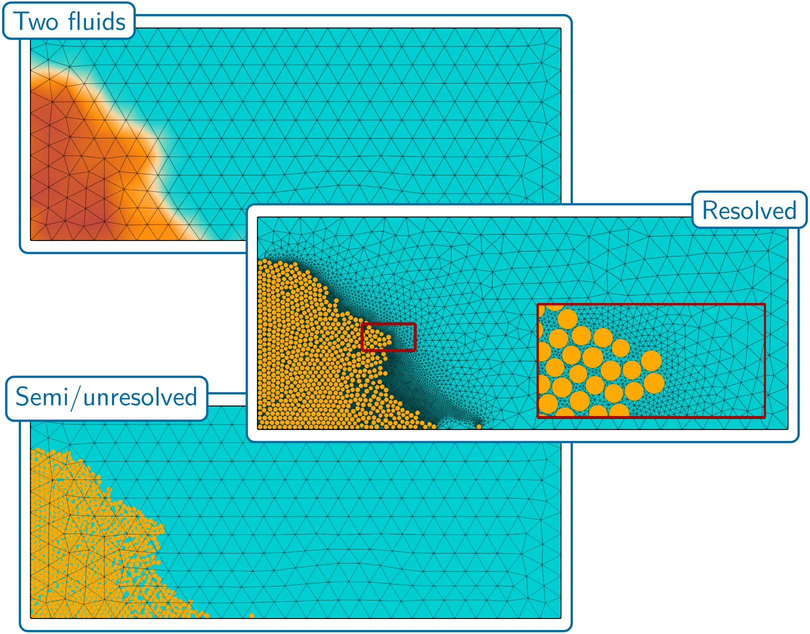
- The grains change the effective viscosity of the mixture:

  $\eta_e = \eta(1 + 2.5\phi_g + 7.6\phi_g^2)^\dagger$, or $\eta_e = \eta(1 - \phi_g/\phi_{gm})^{-n*}$

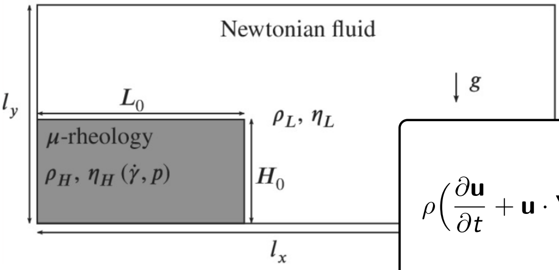
- Non-Newtonian behaviours (even for a Newtonian ambient fluid!):
  - Shear-thinning at constant pressure
  - Shear-thickening at constant volume

†: Batchelor. ∗: Krieger-Dougherty.

The three main approaches



Two fluids models



$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = \nabla\cdot\overbrace{(2\eta\mathbf{d} - p\mathbf{I})}^{\boldsymbol{\sigma}} + \rho\mathbf{g} + \mathbf{f}$$

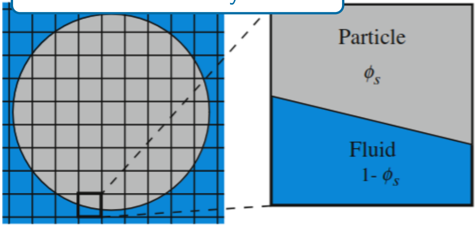
$$\nabla\cdot\mathbf{u} = 0$$

- A constitutive law for the granular material is required
  $\mu(I)$ rheology: $\eta = \mu(I)p/\dot{\gamma}$, $I = \dot{\gamma}d/\sqrt{p/\rho}$
- Fast and easy to implement
- Lack of detail at the grain scale

Gesenhues, L., Behr, M. (2021). Simulating dense granular flow using the $\mu(I)$-rheology within a space-time framework. International Journal for Numerical Methods in Fluids, 93(9), 2889-2904.

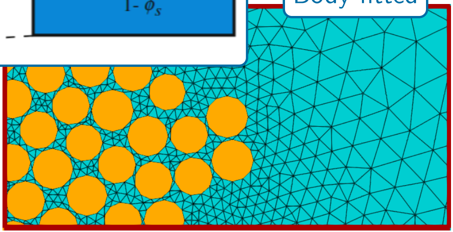
Resolved models

Immersed Boundary method



$$\mathbf{f} = \int_{\Gamma_g} \boldsymbol{\sigma} \cdot \mathbf{n} d\Gamma_g \mathbf{n}$$

Body fitted

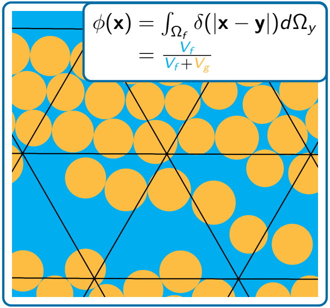


$$\mathbf{f} = \int_{\Gamma_g} \boldsymbol{\sigma} \cdot \mathbf{n} d\Gamma_g \mathbf{n}$$

- The interaction force is directly computed by integrating along the grain boundary
- The mesh size **must** be much smaller than the grains

Washino, K., et al. "Direct numerical simulation of solid–liquid–gas three-phase flow: fluid–solid interaction." Powder technology 206.1-2 (2011): 161-169.

Semi and unresolved models rely on volume-averaged equations



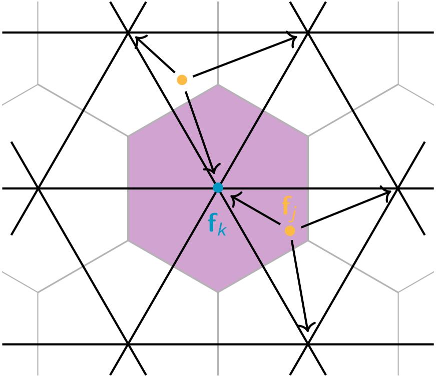
$$\phi(\mathbf{x}) = \int_{\Omega_f} \delta(|\mathbf{x} - \mathbf{y}|) d\Omega_y = \frac{V_f}{V_f + V_g}$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \frac{\rho \mathbf{u}\mathbf{u}}{\phi} = \nabla \cdot \left(2\eta\phi \mathbf{d}\left(\frac{\mathbf{u}}{\phi}\right) - p\mathbf{I}\right) + \mathbf{f} + \phi\rho\mathbf{g}$$

- The averaging kernel $\delta(r)$ is striclty positive and decreasing with r, normalised ($\int_\Omega \delta d\Omega = 1$), and has derivatives of all orders for every r
- Unresolved models use mesh elements as averaging volumes
  - Simple and easy, but mesh size larger than the grains
- Semiresolved models use a larger averaging kernel
  - More flexible mesh size, but boundary treatment nontrivial

The fluid-grain interaction force



$$\mathbf{f}_k = \frac{1}{V_k} \sum_{i=1}^{N} \sum_{j=1}^{N_g} \mathbf{f}_j \tau_i(\mathbf{x}_j)$$

- $\mathbf{f}_i = \overbrace{-V_i \nabla p|_{\mathbf{x}_i}}^{\text{pressure gradient}} - \underbrace{\mathbf{f}_{i,d}}_{\text{drag}}$
- On a single sphere:

$$\mathbf{f}_{i,d} = \underbrace{C_d \frac{\pi d^2}{4} \left|\left| \mathbf{v}_i - \frac{\mathbf{u}}{\phi}|_{\mathbf{x}_i} \right|\right|}_{\gamma_i} \left(\mathbf{v}_i - \frac{\mathbf{u}}{\phi}|_{\mathbf{x}_i}\right)$$

$$C_d = \left(0.63 + \frac{4.8}{\sqrt{Re_i}}\right)^2$$

$$Re_i = \frac{d \rho_f \phi|_{\mathbf{x}_i}}{\eta} \left|\left| \mathbf{u}_i - \frac{\mathbf{v}}{\phi}|_{\mathbf{x}_i} \right|\right|$$

- Taking porosity into account:

$$\mathbf{f}_{i,d} = \phi|_{\mathbf{x}_i} \gamma_i \left(\mathbf{v}_i - \frac{\mathbf{u}}{\phi}|_{\mathbf{x}_i}\right)$$

Time discretisation of the global problem

Grain dynamics

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

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \Delta t \mathbf{v}^{n+1}$$

Contacts

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

$$P_N^{n+1} \geq 0$$

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

Fluid dynamics

$$\frac{\phi^n - \phi^{n-1}}{\Delta t} + \nabla \cdot \mathbf{u}^{n+1} = 0$$

$$\rho\left(\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \nabla \cdot \frac{\mathbf{u}^{n+1}\mathbf{u}^n}{\phi^n}\right) = \nabla \cdot 2\eta\phi^n \mathbf{d}^{n+1} - \phi^n \nabla p^{n+1} + \left(\mathbf{f}^{n+1} + \mathbf{V}_g \nabla p^{n+1}|_{\mathbf{x}^{n+1}}\right) + \phi^n \rho \mathbf{g}$$

- Only explicit couplings are computationally affordable!

  Sadly, they are unstable

A semi-implicit Patankar scheme to the rescue

Grain equation of dynamics

$$\frac{\mathbf{u}_i^* - \mathbf{u}_i^n}{\Delta t} = \mathbf{g} + \frac{1}{m_i}\left(\mathbf{r}_i^n + m\mathbf{g} - V_i \nabla p - \gamma^n \left(\mathbf{u}_i^* - \frac{\mathbf{v}^{n+1}}{\phi^n}\Big|_{\mathbf{x}_i^n}\right)\right)$$

Predicted new grain velocity

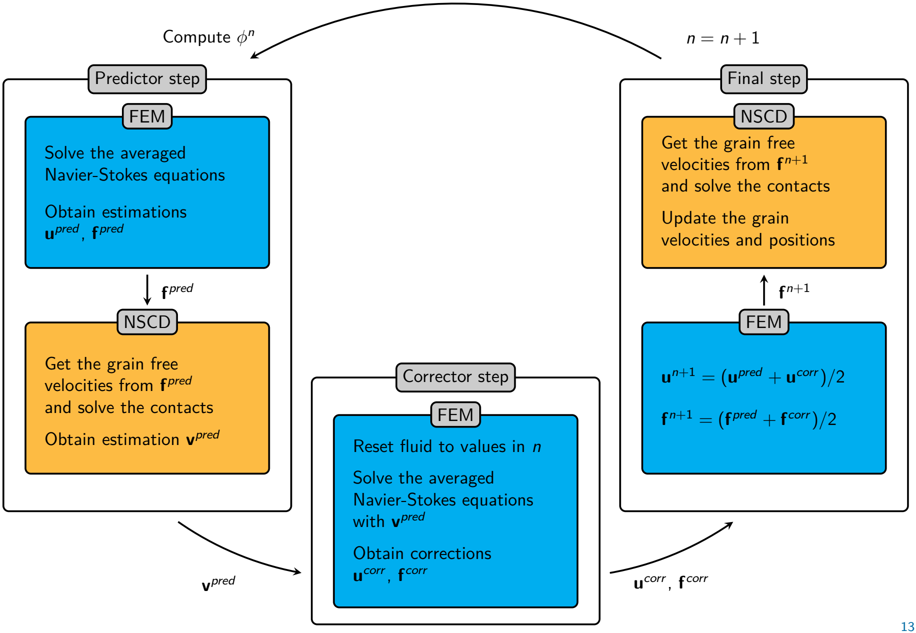
$$\mathbf{u}_i^* = \frac{\Delta t}{m + \gamma^n \Delta t}\left(\frac{m}{\Delta t}\mathbf{u}_i^n + m\mathbf{g} + \mathbf{r}_i^n - V_i \nabla p + \gamma^n \frac{\mathbf{v}^{n+1}}{\phi^n}\Big|_{\mathbf{x}_i^n}\right)$$

Force estimation

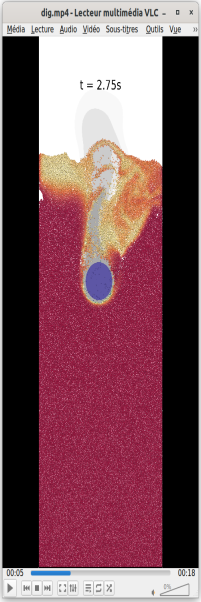
$$\mathbf{f}_i^{n+1} = \gamma^n \left(\mathbf{u}_i^* - \frac{\mathbf{v}^{n+1}}{\phi^n}\Big|_{\mathbf{x}_i^n}\right)$$

- The net contact force $\mathbf{r}_i$ on each grain is computed from its change in velocity after the resolution of the contacts

A stable explicit coupling scheme



Can you feel the heat?



$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \frac{\rho \mathbf{u}\mathbf{u}}{\phi} = \nabla \cdot \left(2\eta\phi \mathbf{d}\left(\frac{\mathbf{u}}{\phi}\right) - p\mathbf{I}\right) + \mathbf{f} + (1 + \beta \Delta T)\phi\rho\mathbf{g}$$

$$\frac{\partial \rho c T}{\partial t} + \mathbf{u} \cdot \frac{\rho c \nabla T}{\phi} = \nabla \cdot (\phi k \nabla T) + q$$

$$m_i \frac{d\mathbf{v}}{dt} = \mathbf{r} - \mathbf{f} + m_i \mathbf{g}$$

$$m_i c \frac{dT}{dt} = Q - Q_f$$

- The correlation for the heat transfer Q_f with the fluid in presence of other grains is inspired from the one for momentum transfer!

Take-home messages

- Immersed granular materials are common and their modelisation is of high interest
- Many different numerical models exist:
  - Two-fluids: cheap but less detailed
  - Resolved models: highly accurate but expensive
  - Semi/unresolved models: grain scale details but affordable
- For semi and unresolved models, empirical fluid grain interaction laws are crucial and their expression
- Care should be given to the explicit coupling to avoid stability issues

What about the project?

- You will receive the exact instructions on Monday May 13, and you will have until Monday June 3 to submit your project on the server
- Your project will consist of the physical analysis of a small application of your choice
- Cases will be proposed in the instructions but you are free to choose another one (in that case you should first ask the teaching staff for validation)
- You are free to simulate your application with smooth DEM or NSCD, and you are free to reuse any part of the solutions of the homeworks on the website
- Your code will not be evaluated for efficiency. You should provide a small README file that describes what your code does and how to run it.
- A bonus will be awarded if you implement an interesting feature seen during the lectures that was not already present in the solutions of the homeworks
- You should write a two pages report describing your application and your results

What about the exam?

- The exam will consist in an interview (approx. 20 min.) about your project
- You are free to prepare a **small** presentation and/or animation(s), but it is not mandatory
- You will be questioned about everything that has been seen during the lectures
- No long mathematical development/demonstration will be required, but you need to understand the underlying concepts behind the math