On the Coupling of Computational Fluid Dynamics with Discrete Element Modelling

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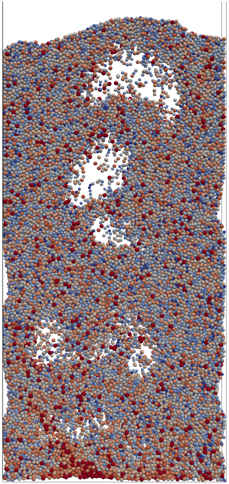
Introduction

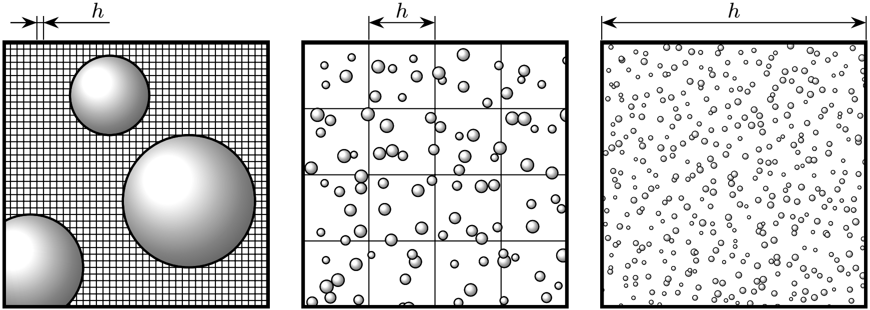
- Discrete Element Modelling (DEM) has become a frequently used tool to analyze particulate processes.
- Computational Fluid Dynamics (CFD) has been a frequently used tool to analyze fluid flow processes.
- Combining the two (CFD-DEM) still has a number of challenges.



Particle-Fluid Flow Coupling

Modelling resolution

There are a number of frameworks to model particulate flows:



Fully resolved

Euler-Lagrange
(CFD-DEM)

Euler-Euler

Particle-Fluid Flow Coupling

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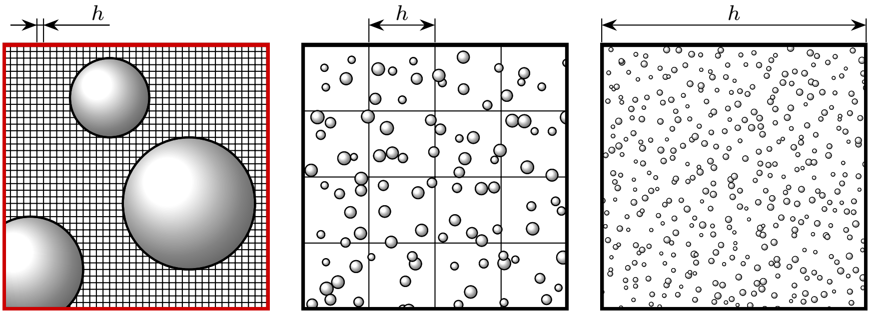

Fully resolved

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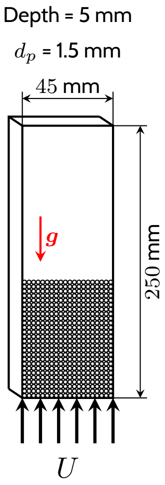
Application to Fluidised Bed

Fully resolved simulation

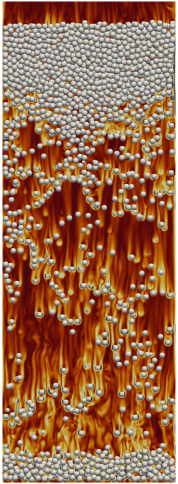


Case setup

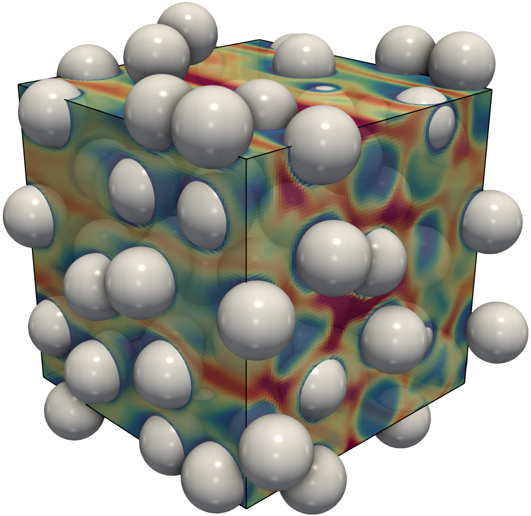
- Based on the experiment of van Wachem *et al.*, *Powder Tech.* 116 (2001), 155-165.
- Inlet superficial velocity

$$U = 0.9\,\mathrm{m.s}^{-1} > U_{\mathrm{mf}} = 0.74\,\mathrm{m.s}^{-1}$$

- Resolution $d_\mathrm{p}/\Delta x = 6.25$
- Particles evolution/collisions modelled with a soft-sphere DEM.



Fully resolved simulations



- The “fully-resolved” methods are very accurate but also very expensive.
- A very high resolution is required for accurate results.
- For practical cases, this is not feasible.

Particulate flow modelling

Modelling resolution

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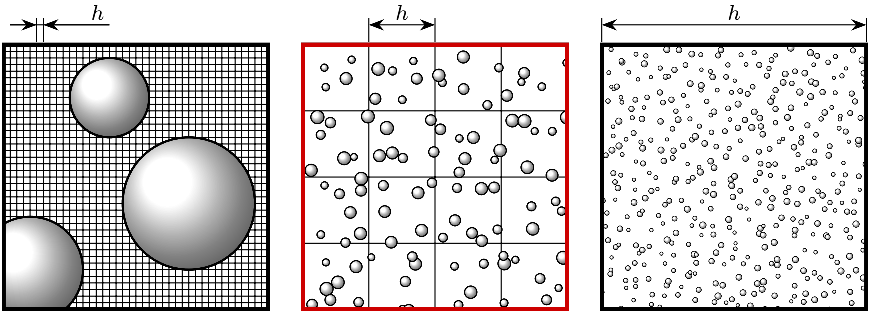

Fully resolved

Euler-Lagrange
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Euler-Euler

Two-way coupled Euler-Lagrange modelling

Governing equations in the dilute regime

Equations of motion of the Eulerian fluid phase

Conservation of mass:

$$\nabla \cdot \mathbf{u}_\mathrm{f} = 0$$

Convervation of momentum:

$$\rho_\mathrm{f} \left[\frac{\partial\ \varepsilon\ \mathbf{u}_\mathrm{f}}{\partial t} + \nabla\ \varepsilon\ \mathbf{u}_\mathrm{f} \mathbf{u}_\mathrm{f} \right] = -\ \varepsilon\ \nabla p + \mu_\mathrm{f}\ \nabla\ \varepsilon\ \nabla \mathbf{u}_\mathrm{f} + \mathbf{M}$$

Equations of motion of a Lagrangian particle

Newton's second law:

$$\rho_\mathrm{p} \frac{\pi\, d_\mathrm{p}^3}{6} \frac{\mathrm{d}\mathbf{v}_\mathrm{p}}{\mathrm{d}t} = \mathbf{F}_\mathrm{p,fluid} + \mathbf{F}_\mathrm{p,body}$$

Maxey-Riley-Gatignol equation:

Maxey & Riley, *Phys. Fluids* (1983)
Gatignol, *J. de Mec. Theor. et Appl.* (1983)

$$\mathbf{F}_\mathrm{p,fluid} = 3\,\pi\,\mu_\mathrm{f}\, d_\mathrm{p}\, f(\mathrm{Re}_\mathrm{p}) \left(\ \tilde{\mathbf{u}}_{\mathrm{f}@\mathrm{p}}\ - \mathbf{v}_\mathrm{p} \right) + \mathbf{F}_\mathrm{p,press} + \mathbf{F}_\mathrm{p,add} + \mathbf{F}_\mathrm{p,hist}$$

Momentum transfer term M

Particle-source-in-cell (PSIC) model:

Crowe, *J. Fluids Eng.* (1977)

$$M = \sum_{\mathrm{p}\,\in\,\mathrm{cell}} -\frac{1}{V_\mathrm{cell}} \left(\mathbf{F}_\mathrm{p,drag} + \mathbf{F}_\mathrm{p,add} + \mathbf{F}_\mathrm{p,hist} \right)$$

Two-way coupled Euler-Lagrange modelling

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Equations of motion of a Lagrangian particle

Newton's second law: $\ldots \mathrm{fluid} + \mathbf{F}_{\mathrm{p,body}}$

Maxey-Riley-Gatignol equation: $\mathbf{F}_{\mathrm{p,fluid}} = \ldots \mathrm{p,add} + \mathbf{F}_{\mathrm{p,hist}}$

Maxey & Riley, *Phys. Fluids* (1983)
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1. ε comes from averaging over particles.

However: this assumes particles and flow are homogeneously distributed in the volume.

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Equations of motion of a Lagrangian particle

Newton's second law: $$\rho_\mathrm{p} \frac{\pi \, d_\mathrm{p}^3}{6} \frac{\mathrm{d}\mathbf{v}_\mathrm{p}}{\mathrm{d}t} = \mathbf{F}_\mathrm{p,fluid} + \mathbf{F}_\mathrm{p,body}$$

Maxey-Riley-Gatignol equation: $$\mathbf{F}_\mathrm{p,fluid} = 3 \, \pi \, \mu_\mathrm{f} \, d_\mathrm{p} \, f(\mathrm{Re}_\mathrm{p}) \left(\tilde{\mathbf{u}}_{\mathrm{f}@\mathrm{p}} - \mathbf{v}_\mathrm{p} \right) + \mathbf{F}_\mathrm{p,press} + \mathbf{F}_\mathrm{p,add} + \mathbf{F}_\mathrm{p,hist}$$

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Momentum transfer term M

Particle-source-in-cell (PSIC) model: $\ldots_\mathrm{p,hist})$ … $\mathrm{p} \in \mathrm{cell}$ … V_cell

Crowe, *J. Fluids Eng.* (1977)

2. $\tilde{\mathbf{u}}_{\mathrm{f}@\mathrm{p}}$ is the undisturbed fluid velocity at p

Definition: the velocity of the (conceptual) flow that is not affected by the particle.

Two-way coupled Euler-Lagrange modelling
The limitations

Problem 1.

Instead of the scalar value of volume fraction, ε, the momentum and drag should take the local *particle assembly structure* into account. This is the topic of our recent research project, but because of time I will not present details here.

Two-way coupled Euler-Lagrange modelling

The limitations

Problem 2.

The velocity available on the Eulerian grid is the disturbed velocity, $\mathbf{u}_\mathrm{f}$, **not** the undisturbed velocity, $\tilde{\mathbf{u}}_\mathrm{f}$.

Two-way coupled Euler-Lagrange modelling

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What we know

- If we approximate $\tilde{\mathbf{u}}_{\mathrm{f}@\mathrm{p}} \simeq \mathbf{u}_{\mathrm{f}@\mathrm{p}}$ when calculating $\mathbf{F}_\mathrm{fluid}$, **as is done in most CFD codes**, an error is introduced!
- This error relates to the magnitude of velocity disturbance induced by the particle:

$$\mathbf{u}'_{\mathrm{f}@\mathrm{p}} = \mathbf{u}_{\mathrm{f}@\mathrm{p}} - \tilde{\mathbf{u}}_{\mathrm{f}@\mathrm{p}}$$

- The magnitude of the self-induced disturbance increases together with the ratio d_p/h (particle diameter/mesh spacing).
- That is why particles are required to be much smaller than the mesh spacing: $d_\mathrm{p} \ll h$.

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How large is the error?

Self-induced velocity disturbance

Governing equations

We limit ourselves to dilute gas-solid flow (relevant to many industrial processes):

- **Gas-solid flow:** $\rho_\mathrm{p} \gg \rho_\mathrm{f} \quad \Rightarrow \quad \mathbf{F}_{\mathrm{p,fluid}} \simeq \mathbf{F}_{\mathrm{p,drag}}$
- **Dilute regime:** particle-particle interactions (collisions + scaling of drag force with volume-fraction) are neglected.

Governing equations for the velocity disturbance induced by a particle p

Substituting $\mathbf{u}_\mathrm{f} = \mathbf{u}'_\mathrm{f} + \tilde{\mathbf{u}}_\mathrm{f}$ in the governing equations for the Eulerian phase, we obtain:

Conservation of mass:

$$\nabla \cdot \mathbf{u}'_\mathrm{f} = 0$$

Conservation of momentum:

$$\rho_\mathrm{f} \left[\frac{\partial \mathbf{u}'_\mathrm{f}}{\partial t} + \tilde{\mathbf{u}}_\mathrm{f} \cdot \nabla \mathbf{u}'_\mathrm{f} + \mathbf{u}'_\mathrm{f} \cdot \nabla \left(\mathbf{u}'_\mathrm{f} + \tilde{\mathbf{u}}_\mathrm{f} \right) \right] = -\nabla p' + \mu_\mathrm{f} \, \Delta \mathbf{u}'_\mathrm{f} - \delta(\mathbf{x} - \mathbf{x}_\mathrm{p}) \, \mathbf{F}_{\mathrm{p,drag}}$$

Discrete Dirac delta function

δ is the Dirac delta function. In the PSIC model, it is approximated as:

Crowe, *J. Fluids Eng.* (1977)

$$\delta(\mathbf{x} - \mathbf{x}_\mathrm{p}) = \begin{cases} 1/V_{\mathrm{cell}} & \mathbf{x}_\mathrm{p} \in \text{cell} \\ 0 & \text{elsewhere} \end{cases}$$

Self-induced velocity disturbance

Estimating the magnitude of the velocity disturbance from the Oseenlet

The magnitude of the averaged self-induced velocity disturbance reads as

Averaged velocity disturbance in a volume similar to that of a computational cell

$$\bar{\mathbf{u}}'_{\mathrm{f}} = \pi\,\alpha^2\,\hat{d}_{\mathrm{p}}\,\Psi_{\mathrm{Oseen}}\left(\mathrm{Re}_{\mathrm{p}},\hat{d}_{\mathrm{p}}\right)\mathbf{u}_\infty, \qquad \alpha = (3/(4\,\pi))^{1/3}, \qquad \hat{d}_{\mathrm{p}} = d_{\mathrm{p}}/h$$

$$\Psi_{\mathrm{Oseen}}\left(\mathrm{Re}_{\mathrm{p}},\hat{d}_{\mathrm{p}}\right) = 3\,\hat{d}_{\mathrm{p}}\,f(\mathrm{Re}_{\mathrm{p}})\left((\alpha\,\mathrm{Re}_{\mathrm{p}})^{-1} - 2\,\hat{d}_{\mathrm{p}}\,(\alpha\,\mathrm{Re}_{\mathrm{p}})^{-2} + 2\,\hat{d}_{\mathrm{p}}^2\,(\alpha\,\mathrm{Re}_{\mathrm{p}})^{-3}\left(1-\exp\left(-\frac{\mathrm{Re}_{\mathrm{p}}\,\alpha}{\hat{d}_{\mathrm{p}}}\right)\right)\right)$$

Evrard, Denner, van Wachem, *Int. J. Multiph. Flow*, 135, 103535 (2021)

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In the Stokes limit

In the Stokes limit (no inertia):

$$\lim_{\mathrm{Re}_\mathrm{p}\to 0}\Psi_\mathrm{Oseen}\left(\mathrm{Re}_\mathrm{p},\hat{d}_\mathrm{p}\right) = 1$$

so the averaged self-induced velocity disturbance is

$$\bar{\mathbf{u}}'_\mathrm{f} = \pi\,\alpha^2\,\hat{d}_\mathrm{p}\,\mathbf{u}_\infty \quad\Rightarrow\quad \bar{\mathbf{u}}'_\mathrm{f} \simeq \frac{6}{5}\,\hat{d}_\mathrm{p}\,\mathbf{u}_\infty$$

Validation

Comparison with numerical results

How well can this predict what happens in two-way coupled EL simulations?

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Let us put the derived expression to test:

We consider a single, isolated, fixed particle subject to a uniform flow $\mathbf{u}_\infty$.

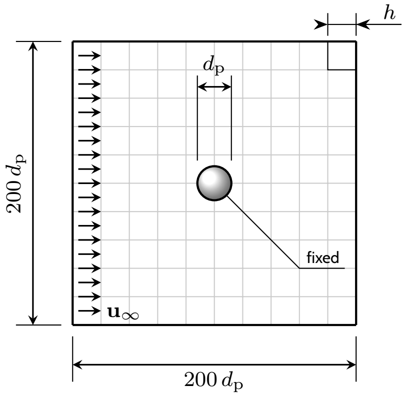
We measure the self-induced disturbance at p as

$$\mathbf{u}'_{\mathrm{f}@\mathrm{p}} = \mathbf{u}_{\mathrm{f}@\mathrm{p}} - \mathbf{u}_\infty$$

where $\mathbf{u}_{\mathrm{f}@\mathrm{p}}$ is interpolated from the Eulerian velocity field.

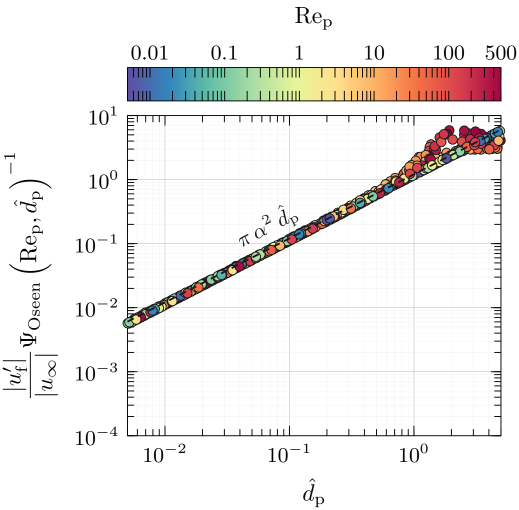
The flow/simulation parameters are randomly selected as

- $\hat{d}_\mathrm{p} = d_\mathrm{p}/h \in [0.005, 5]$
- $\mathrm{Re}_\mathrm{p} = u_\infty \, d_\mathrm{p} \, \rho_\mathrm{f}/\mu_\mathrm{f} \in [0.005, 500]$



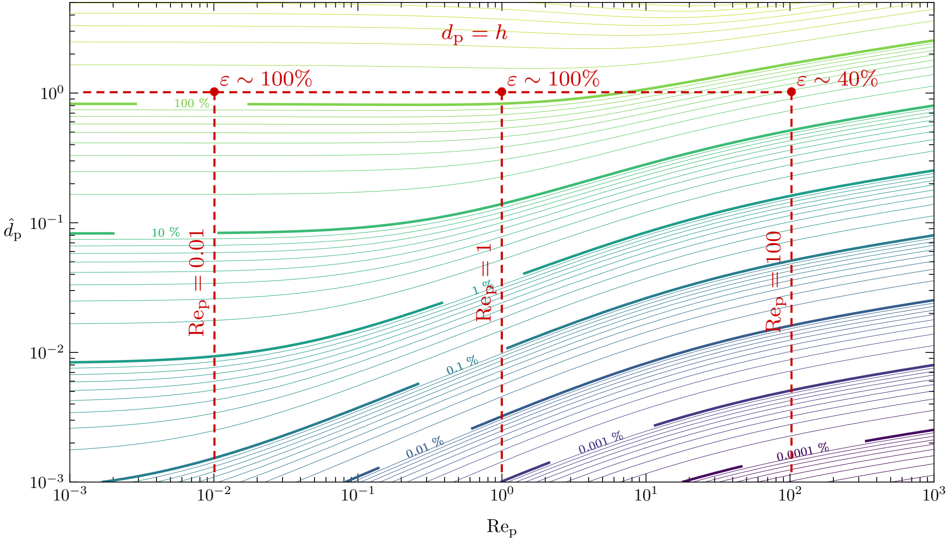
Validation

After 800 numerical experiments with random flow/simulation parameters



Error map

A graphical tool to estimate the errors to be expected



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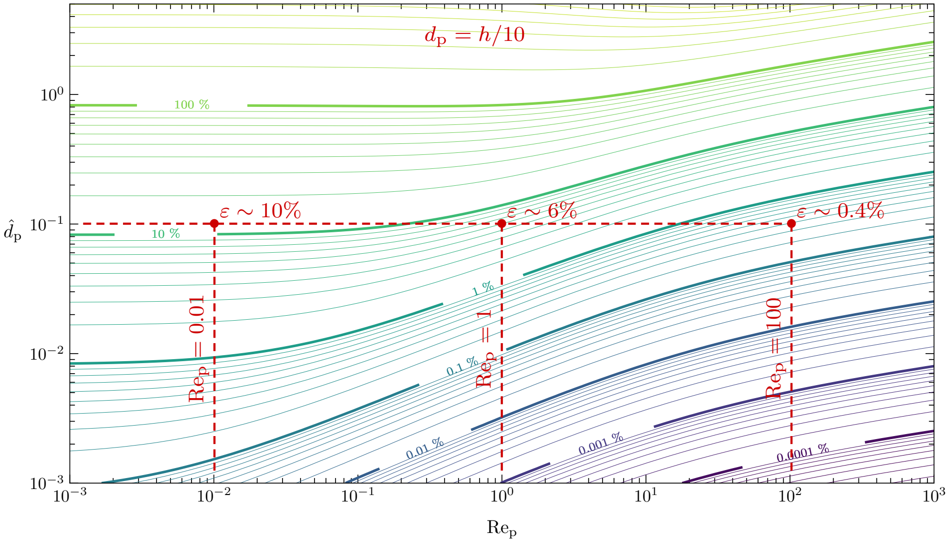

Conclusions

So far

When simulating dilute gas-solid flows with the particle-source-in-cell Euler-Lagrange method:

- **An error is made** when estimating the undisturbed flow velocity from the Eulerian velocity field.
- This error depends on the **particle Reynolds number**, and the **ratio of particle size/mesh spacing**.
- In the Stokes regime, this relative error is:

$$\mathrm{Error} \sim \frac{6}{5}\frac{d_\mathrm{p}}{h}$$

- More generally, this relative error is approximated as:

$$\mathrm{Error} \sim \left(\frac{3\sqrt{\pi}}{4}\right)^{2/3} \frac{d_\mathrm{p}}{h}\,\Psi_\mathrm{Oseen}\left(\mathrm{Re}_\mathrm{p}, \frac{d_\mathrm{p}}{h}\right)$$

- For example: With the classical recommendation $d_\mathrm{p} \lesssim h/10$, errors of up to 10% can still be made!

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- For example: With the classical recommendation $d_\text{p} \lesssim h/10$, errors of up to 10% can still be made!
- ***Can we get rid of these errors?***

Estimating and subtracting the self-induced velocity disturbance

As done previously for the PSIC model, we can estimate the self-induced disturbance in the low Reynolds number limit by solving:

Oseen's equations

Conservation of mass: $\nabla \cdot \mathbf{u}'_\mathrm{f} = 0$

Conservation of momentum: $\rho_\mathrm{f}\, \mathbf{u}_\infty \cdot \nabla \mathbf{u}'_\mathrm{f} = -\nabla p' + \mu_\mathrm{f}\, \Delta \mathbf{u}'_\mathrm{f} - k(\|\mathbf{x} - \mathbf{x}_\mathrm{p}\|)\, \mathbf{F}_{\mathrm{p,drag}}$

Using the Wendland kernel, the regularised Stokeslet velocity along the direction of $\mathbf{F}_{\mathrm{p,drag}}$ reads as:

$$u'_\mathrm{f}(\hat{r}, \theta, \phi) = \frac{-F_{\mathrm{p,drag}}}{120\, \mu_\mathrm{f}\, \delta\, \pi\, \hat{r}^3} \begin{cases} (63\, \hat{r}^{10} - 300\, \hat{r}^9 + 525\, \hat{r}^8 - 360\, \hat{r}^7 + 84\, \hat{r}^5) \sin(\theta)^2 \cos(\phi)^2 \\ \quad - 81\, \hat{r}^{10} + 400\, \hat{r}^9 - 735\, \hat{r}^8 + 540\, \hat{r}^7 - 168\, \hat{r}^5 + 60\, \hat{r}^3 & \text{if } 0 \le \hat{r} \le 1 \\ (15\, \hat{r}^2 - 3) \sin(\theta)^2 \cos(\phi)^2 + 15\, \hat{r}^2 + 1 & \text{if } \hat{r} > 1 \end{cases} .$$

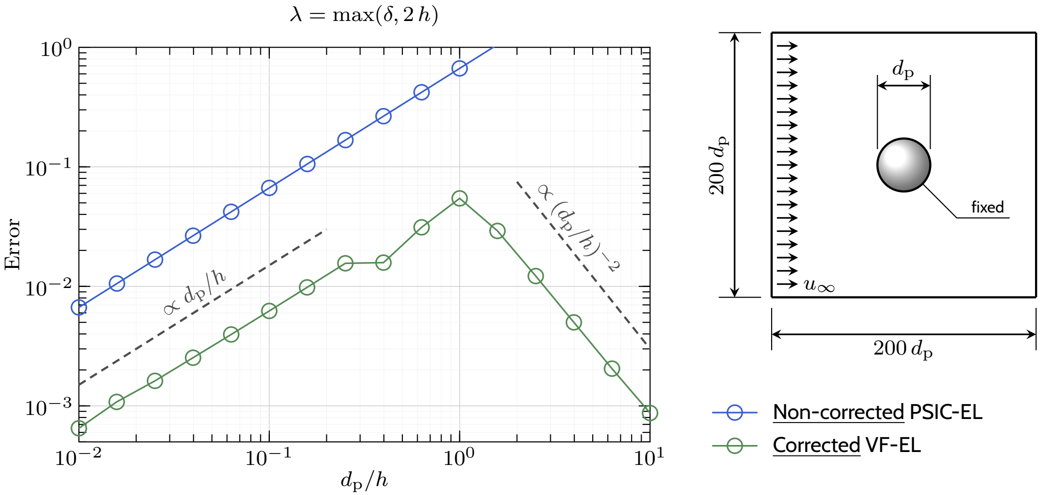
where $\hat{r} = r/\delta$.

Undisturbed velocity recovery at p

$$\tilde{\mathbf{u}}_{\mathrm{f}@\mathrm{p}} = \mathbf{u}_{\mathrm{f}@\mathrm{p}} + \frac{\mathrm{F}_{\mathrm{p,drag}}}{2\, \pi\, \mu_\mathrm{f}\, \delta}$$

Estimating the self-induced velocity disturbance

Flow through the source field of a fixed particle with $\mathrm{Re_p} = 0.01$

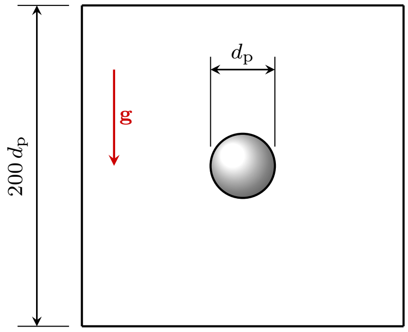


Validation

Test on a particle settling under gravity

We now have a recipe for recovering the undisturbed velocity in VF-EL!

Let us put it to test.

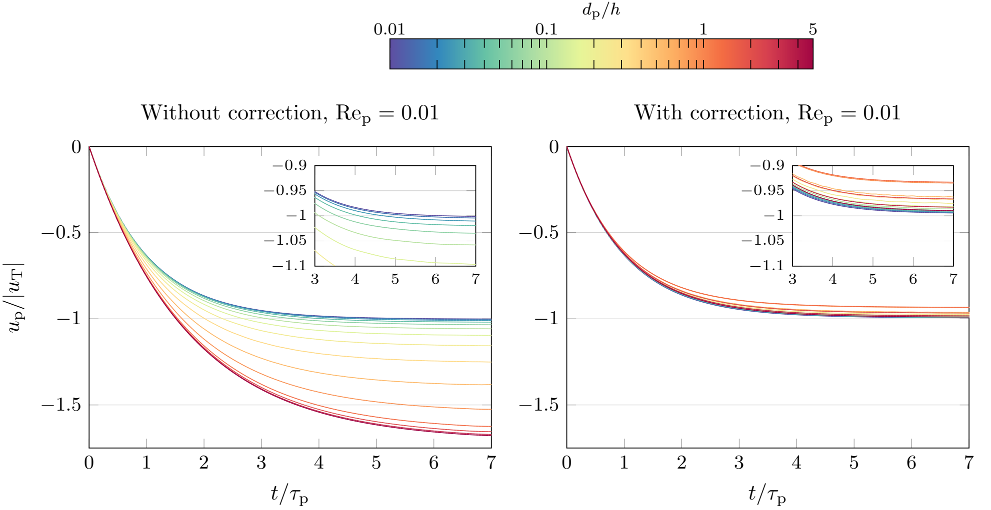


Case setup

- Non-corrected/corrected averaged flow velocity is used for drag.
- $\mathrm{Re}_\mathrm{p} \in [0.01, 100]$
- $d_\mathrm{p}/h \in [0.01, 5]$

Validation

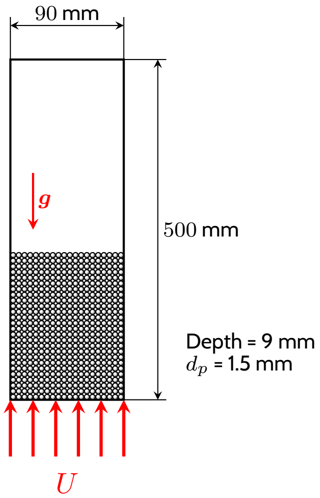
Test on a settling particle



Evrard, Denner, van Wachem, *J. Comp. Phys. X*, 8, 100078 (2020)

Application to a fluidised bed

Case setup

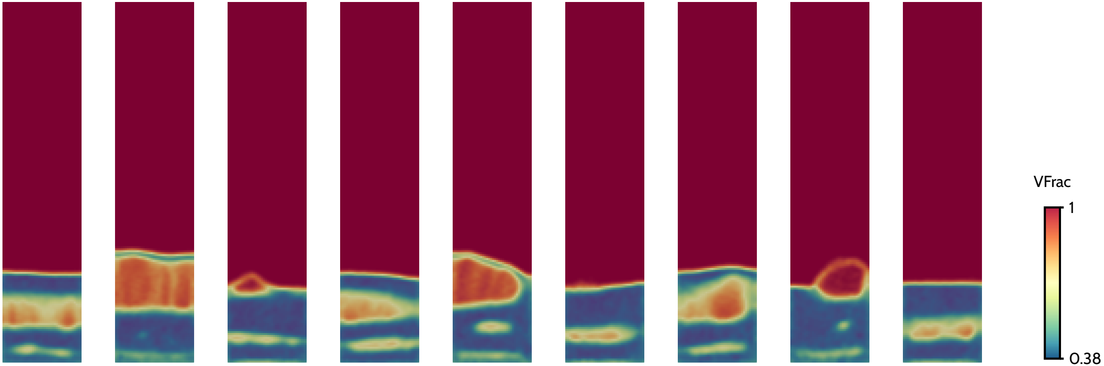


Case setup

- Based on van Wachem *et al.*, Powder Technology 2001
- Inlet superficial velocity $U = 0.8$ m.s^{-1}
- Filter size $\delta = 3\ d_p$
- Particle size $d_p = (2/3)\ \Delta x$
- Total of ~ 20000 particles
- Particles are mirrored at the boundaries to guarantee convervative filtering of quantities
- Particles evolution modelled with a soft-sphere DEM

Application to a fluidised bed

$\delta/d_p = 3$, $d_p/\Delta x = 2/3$, ~ 20000 particles



$t = 1.00$ s $t = 1.13$ s $t = 1.25$ s $t = 1.38$ s $t = 1.50$ s $t = 1.63$ s $t = 1.75$ s $t = 1.88$ s $t = 2.00$ s

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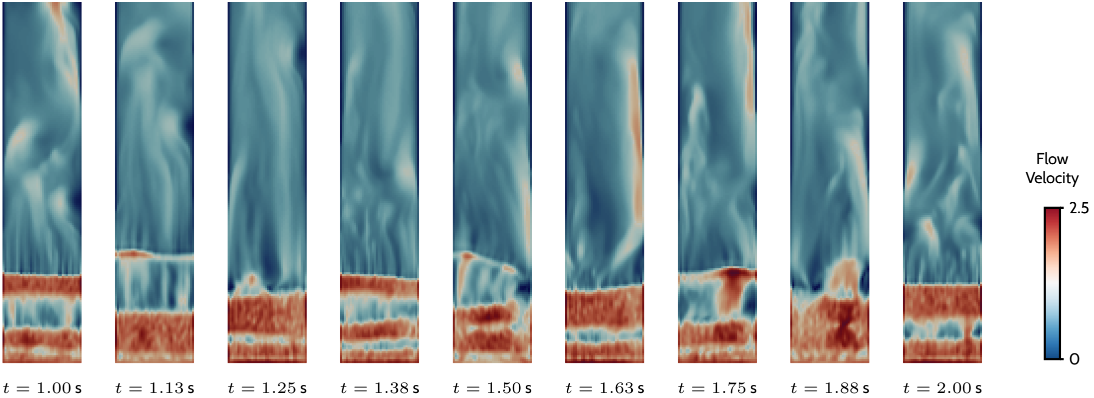

Conclusions

- The relative error for 'standard' CFD-DEM, particle-source-in-cell Euler-Lagrange, is:

$$\text{Error} \sim \frac{6}{5}\frac{d_\text{p}}{h}$$

To improve this, we have proposed a **Volume-Filtered Euler-Lagrange method with velocity correction**:

- The momentum transfered from Lagragian particles to the Eulerian fluid is **regularised** with a smooth kernel whose length scale relates to the particle diameter.
- The self-induced particle velocity disturbance is **estimated** and **substracted** from the interpolated velocity.
- The resulting approach **converges with mesh refinement** (unlike classical CFD-DEM, PSIC-EL).
- The framework allows for optimised mesh configurations (*e.g.*stretched meshes, AMR, complex geometries)
- Work in progress:
  - Extension to flows in the dense regime (structure in ε)