Simulation of Granular Two-phase flow

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Simulation of Granular Two-phase flow

Important example: gas fluidized beds
Three basic models for two-phase granular flow:

- DNS
- DEM
- TFM

Euler Lagrange
Euler Lagrange
Euler Euler
Outline

I. DNS models for granular two-phase flow

II. DEM models for granular two-phase flow

III. Example: Vibrated granular beds
I. DNS models for granular two-phase flow

Three issues:

- How to model the particles?
- How to model the fluid phase?
- How to model the fluid-particle interaction?
I. DNS models for granular two-phase flow

1. Models for the solid phase

2. Models for the fluid phase (CFD, LBM)

3. Fully resolved fluid-particle interaction
1. Models for the **solid** phase

- Phase consists of individual particles $\rightarrow$ Lagrangian

- Methods borrowed from classical “molecular dynamics”

- Two different methods  
  A. Soft-sphere model  
  B. Hard-sphere model
1A. Solid Phase Models: Soft-Sphere

Position of particle \( a \): \( \mathbf{R}_a \)

Newton’s equation of motion:

\[
M \frac{d^2 \mathbf{R}_a}{dt^2} = \mathbf{F}_{a,tot}
\]

is integrated numerically:

\[
\mathbf{R}_a(t + \delta t) = 2\mathbf{R}_a(t) - \mathbf{R}_a(t - \delta t) + \frac{\mathbf{F}_{a,tot}(t)}{M} \delta t^2
\]

total force:

\[
\mathbf{F}_{a,tot} = \sum_b \mathbf{F}_{ab} + Mg
\]

→ Time driven scheme

→ Interaction force \( \mathbf{F}_{ab} \) follows from a continuous potential

→ “soft-sphere model”
1A. Solid Phase Models: Soft Sphere

Interaction force: \[ F_{ab} = F_{coll}^{ab} + F_{el}^{ab} + F_{coh}^{ab} \]

- Collision force: Spring-dashpot model
  \[ F_{coll, n}^{ab} = -k \delta n_{ab} - \eta v_{ab, n} \]
  - spring constant
  - damping coefficient

- Electrostatic force
  \[ F_{el}^{ab} = -\frac{q^2}{4\pi\varepsilon} \frac{n_{ab}}{R_{ab}^2} \]

- Cohesive force
  \[ F_{coh}^{ab} = \frac{Ad}{6} \frac{n_{ab}}{S_{ab}^2} \]
1A. Solid Phase Models: Soft-Sphere

\[ \mathbf{R}_a(t), \mathbf{V}_a(t) \]

soft-sphere model

Coulomb force etc.

\[ \mathbf{F}_{ab}^{\text{coll.}} \]

\[ M \ddot{\mathbf{R}}_a = \sum_b \mathbf{F}_{ab}^{\text{coll.}} \]

\[ \mathbf{R}_a(t + \delta t), \mathbf{V}_a(t + \delta t) \]
1B. Solid Phase Models: Hard-sphere

**Simplified MD: hard-sphere model**

- Collision time between spheres can be calculated analytically:

\[
    t_{ab} = \frac{-R_{ab} \cdot V_{ab} - \sqrt{(R_{ab} \cdot V_{ab})^2 - V_{ab}^2 \left[ R_{ab}^2 - 4R^2 \right]}}{V_{ab}}
\]

- Evolution in time: free-flight to nearest collision event followed by instantaneous binary collision (event driven scheme)

- Collision: change of momentum does not follow from forces, but is calculated via:

\[
    \Delta \vec{v}_a = \left( \frac{1+e}{2} \right) \frac{R_{ab} \cdot V_{ab}}{4R^2} R_{ab}
\]
Advantages of hard-sphere over soft-sphere

- Much faster for dilute systems
- Soft potential often “too soft” to model e.g. glass spheres

Disadvantages of hard-sphere over soft-sphere

- HS breaks down for dense (close packed) systems
- Update not based on forces: more difficult to include other interactions
Outline

1. Models for the solid phase
2. Models for the fluid phase (CFD, LBM)
3. Fully resolved fluid-particle interaction
2. Models for the **fluid** phase (CFD, LBM)

- Continuum description of the phase → Eulerian
- Time evolution governed by Navier-Stokes (NS) equation
- Two basic methods for solving the NS equations on a grid
  
  A. Computational Fluid Dynamics
  B. Lattice Boltzmann Method
2. Fluid Phase Models: Computational Fluid Dynamics (CFD)

Basic idea: solve the set of differential equations:

$$\nabla \cdot u = 0$$

$$\partial_t u = -\frac{1}{\rho} \nabla P - \nabla \cdot uu - \nabla \cdot \tau$$

by finite difference methods

Closures for $P$ and $\tau$

$$P = \frac{RT}{M} \rho$$

$$\tau = -(\lambda - \frac{2}{3} \mu)(\nabla \cdot u) I + \mu((\nabla u) + (\nabla u)^T)$$
2. Fluid Phase Models: Computational Fluid Dynamics (CFD)

\[ \nabla \cdot \mathbf{u} = 0 \]

\[ \partial_t \mathbf{u} = -\frac{1}{\rho} \nabla P - \nabla \cdot \mathbf{uu} - \nabla \cdot \mathbf{\tau} \]

\[ \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\delta t} = -\frac{1}{\rho} \nabla P^{n+1} - \left[ \nabla \cdot \mathbf{uu} + \nabla \cdot \mathbf{\tau} \right]^n \]

finite diff. form

\[ \mathbf{u}^{n+1} = \mathbf{u}^n - \frac{\delta t}{\rho} \nabla P^{n+1} - \delta t \mathbf{A}^n \]

\[ \hat{\mathbf{u}}^{n+1} = \mathbf{u}^n - \frac{\delta t}{\rho} \nabla \hat{P}^{n+1} - \delta t \mathbf{A}^n \]

tentative velocity

\[ -\mathbf{u}^{n+1} + \hat{\mathbf{u}}^{n+1} = \frac{\delta t}{\rho} \nabla \left[ \Phi^{n+1} - \hat{P}^{n+1} \right] \]

\[ \Phi = P^{n+1} - \hat{P}^{n+1} \]

taking \( \nabla \cdot \)

\[ -\nabla \cdot \mathbf{u}^{n+1} + \nabla \cdot \hat{\mathbf{u}}^{n+1} = \frac{\delta t}{\rho} \nabla^2 \Phi \]

\[ P^{n+1} = \hat{P}^{n+1} + \Phi \]

\[ \mathbf{u}^{n+1} = \hat{\mathbf{u}}^{n+1} + \frac{\delta t}{\rho} \nabla \Phi \]
Initial guess:

\[ \hat{p}^{n+1} \Rightarrow \nabla \hat{p}^{n+1} \]

Solution procedure to calculate variables at time \( n+1 \)

\[ \hat{u}^{n+1} = u^n - \frac{\delta t}{\rho} \nabla \hat{p}^{n+1} - \delta t A^n \]

\[ \nabla \cdot \hat{u}^{n+1} = \frac{\delta t}{\rho} \nabla^2 \Phi \]

\[ p^{n+1} = \hat{p}^{n+1} + \Phi \]

\[ u^{n+1} = \hat{u}^{n+1} + \frac{\delta t}{\rho} \nabla \Phi \]
Finite differences in space: requires discretization of space
Divide space up in cells of $\delta l \cdot \delta l \cdot \delta l$
Define $P_{ijk}$ as the pressure at the center of the cell $\{i, j, k\}$

Then for instance
\[
\left( \frac{dP}{dx} \right)_{i+\frac{1}{2},j,k} = \frac{P_{i+1,j,k} - P_{i,j,k}}{\delta l}
\]

Note: velocity is calculated from an equation like:
\[
\mathbf{u}^{n+1} = \mathbf{u}^n - \frac{\delta t}{\rho} \nabla P^{n+1} - \frac{\delta t}{\rho} \mathbf{A}^n
\]

→ Requires that velocities are defined at the faces of the cell

\[
[u_x]_{i+\frac{1}{2},j,k} \quad [u_y]_{i,j+\frac{1}{2},k} \quad [u_z]_{i,j,k+\frac{1}{2}}
\]

Then for instance
\[
\left( \frac{du_x}{dx} \right)_{i,j,k} = \frac{u_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k}}{\delta l}
\]
is again defined at the cell center
Staggered grid

Define scalar variables at the cell centers, vector variables at the cell faces

- scalar variables $P$, $\rho$
- $x$-velocity component $u_x$
- $y$-velocity component $u_y$
- $z$-velocity component $u_z$
Resolution in time and space set by $\delta t, \delta l$

Any instability will originate from the explicit term in the velocity update

$$u^{n+1} = u^n - \frac{\delta t}{\rho} \nabla P^{n+1} - \frac{\delta t}{\rho} A^n$$

$A = \nabla \cdot \rho uu + \nabla \cdot \tau$

Stability condition from explicit treatment of

i) Convective term: $u_x + u_y + u_z < \frac{\delta l}{\delta t}$  \hspace{1cm} (Courant)

ii) Stress term: $6 \nu < \frac{(\delta l)^2}{\delta t}$
2. Fluid Phase Models: Lattice Boltzmann Method (LBM)

Hydrodynamic variables for the gas phase: \( \rho(r) \) and \( u(r) \)

These 4 variables can be captured by 1 variable: \( f(r, c) \)

\[
\int dc \ f(r, c) = \rho(r) \\
\int dc \ c \ f(r, c) = \rho(r)u(r)
\]

Time evolution of \( f(r, c) \): the Boltzmann Equation (BE)

\[
\partial_t f + c \cdot \nabla f = C(f) \quad \text{where} \quad C(f) = -\frac{f - f_{eq}(\rho, u)}{\tau}
\]

\[
\int dc \quad \Rightarrow \quad \partial_t \rho + \nabla \cdot (\rho u) = 0
\]

\[
\int dc \ c \quad \Rightarrow \quad \partial_t (\rho u) + \nabla \cdot (\rho uu) = -\nabla p - \nabla \cdot \tau
\]
Discretization of coordinate and velocity space

\[ f(r, c) \rightarrow f_i(r) \]

\( r \) restricted to lattice sites

\[ \downarrow \]

discrete velocities \( c_i \), such that \( r + c_i \delta t \) is located on a neighboring lattice site

For the 2-D square lattice:

4 velocities:

\[ \{c_1, c_2, c_3, c_4\} \]

\[ |c_i| = \frac{\delta l}{\delta t} \]
2. Fluid Phase Models: Lattice Boltzmann Method (LBM)

**Continuous**

\[
\begin{align*}
\rho(r,t) &= \int dc \, f(r,c,t) \\
\rho(r,t) \, u(r,t) &= \int dc \, c \, f(r,c,t)
\end{align*}
\]

\[
\partial_t f + c \cdot \nabla f = C(f)
\]

\[
C(f) = -\frac{f - f^{eq}(\rho, u)}{\tau}
\]

**Discrete**

\[
\begin{align*}
\rho(r,t) &= \sum_i f_i(r,t) \\
\rho(r,t) \, u(r,t) &= \sum_i c_i \, f_i(r,t)
\end{align*}
\]

\[
f_i(r + c_i \delta t, t + \delta t) = f_i(r,t) + C_i
\]

\[
C_i = -\frac{f_i - f_i^{eq}(\rho, u)}{\tau}
\]

\[
f_i^{eq} = \rho \, e^{-(c_i - u)^2/c_s^2}
\]
Update in lattice-Boltzmann scheme:

\[ \rho \mathbf{u} = \sum_i c_i f_i \]
\[ \rho = \sum_i f_i \]

\[ f_i^*(\mathbf{r}, t) = f_i(\mathbf{r}, t) - \frac{1}{\tau} \left[ f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t) \right] \]

\[ f_i(\mathbf{r} + c_i \delta t, t + \delta t) = f_i^*(\mathbf{r}, t) \]

No iterations
All calculations are local
Advantages Lattice-Boltzmann:
- Easy to program
- Ideally suited for parallelization
- Simple boundary conditions
- Faster than CFD?

Disadvantages Lattice-Boltzmann:
- Stability conditions not as clear as in CFD
- Conversion to SI units is less straightforward
- Not straightforward to include heat transfer, and/or GLS flow
Outline

1. Models for the solid phase

2. Models for the fluid phase (CFD, LBM)

3. Fully resolved fluid-particle interaction
3. Fully-resolved fluid-particle interaction

Interaction between solid and fluid: no-slip boundary condition

LBM or CFD
3. Fully resolved fluid-particle interaction: LBM

Resolved flow with **LBM**: Bounce Back at boundary nodes

Define boundary node as point halfway an exterior and interior lattice site

In the propagation step: distribution “bounces back” at boundary nodes, and returns to its original site → average flow velocity is zero at boundary site
Update with boundary rules

Fluid phase:

\[ f_i(t) \rightarrow \rho, \mathbf{u} \rightarrow f_i^{eq} \rightarrow f_i^* = f_i(t) - \frac{1}{\tau} [f_i(t) - f_i^{eq}] \rightarrow f_i(t + \delta t) = \text{propagated} \ f_i^* \ \text{with bounce-back at bn} \]

Solid phase:

\[ R_a(t), V_a(t) \rightarrow \text{boundary nodes (bn) + velocities} \]

output

\[ f \rightarrow \text{p force} \ F_{f,a} \]

\[ M\ddot{R}_a = \sum_b F_{ab}^{\text{coll.}} + F_{f,a} \]

\[ R_a(t + \delta t), V_a(t + \delta t) \]
3. Fully resolved fluid-particle interaction: LBM

Fluid-particle force for a (infinite) random array (Stokes flow)

vdH, Beetstra & Kuipers, JFM 2005

\[ F(\phi) = \frac{F_{f,p}}{3\pi \mu du} = \frac{10\phi}{(1-\phi)^2} + \frac{1+1.5\phi^{1/2}}{(1-\phi)^{-2}} \]

Relations have also been obtained for general Re and polydisperse systems
3. Fully resolved fluid-particle interaction: CFD

Interaction between solid and gas: stick boundary condition at surface

CFD
Define marker point on the surface, each of which applies a force $F_m$ on the fluid, such that the velocity $u_m$ of the fluid at the marker point is equal to the surface velocity $w_m$.

$$F_m = C \delta l^3 \cdot \frac{\rho}{\delta t} (w_m - \tilde{u}_m)$$

Velocity from update without forcing

$$C = \frac{4\pi}{N} \left( \frac{R}{\delta l} \right)^2$$
Force at marker point location:

\[ \mathbf{F}_m = C \delta l^3 \cdot \frac{\rho}{\delta t} (\mathbf{w}_m - \mathbf{\tilde{u}}_m) \]

Total force density at \( \{ijk\} \) from all force points in range of \( \{ijk\} \)

Update flow field on Eulerian grid:

\[ \mathbf{u}^{n+1}_{ijk} = \mathbf{u}^n_{ijk} - \frac{\delta t}{\rho} (\nabla P^{n+1})_{ijk} - \frac{\delta t}{\rho} \mathbf{A}^n_{ijk} + \frac{\delta t}{\rho} \mathbf{f}_{ijk} \]

Required: Mapping

Lagrange \( \rightarrow \) Euler

Euler \( \rightarrow \) Lagrange

\[(\text{note: for simplicity, we assume that the velocity is defined on gridpoints } ijk \text{ (no staggered grid)})\]
3. Fully resolved fluid-particle interaction: CFD

Euler → Lagrange mapping: Volume weighing

Basic idea shown in 2-D (surface weighing)

\[
F_m = C \delta l^3 \cdot \frac{\rho}{\delta t} (w_m - \tilde{u}_m)
\]

\[
\tilde{u}_m = \frac{N}{S_1} \tilde{u}_{i,j,k} + \frac{N}{S_2} \tilde{u}_{i+1,j,k} + \frac{N}{S_3} \tilde{u}_{i+1,j+1,k} + \frac{N}{S_4} \tilde{u}_{i,j+1,k}
\]

\[
\frac{N}{S_1} + \frac{N}{S_2} + \frac{N}{S_3} + \frac{N}{S_4} = 1
\]
3. Fully resolved fluid-particle interaction: CFD

Lagrange $\rightarrow$ Euler mapping: Volume weighing
Basic idea shown in 2-D (surface weighing)

\[
\begin{align*}
\mathbf{f}_{i,j,k} &= \frac{N}{S_1} \cdot \frac{\mathbf{F}_m}{\delta l^3} \\
\mathbf{f}_{i+1,j,k} &= \frac{N}{S_2} \cdot \frac{\mathbf{F}_m}{\delta l^3} \\
\mathbf{f}_{i+1,j+1,k} &= \frac{N}{S_3} \cdot \frac{\mathbf{F}_m}{\delta l^3} \\
\mathbf{f}_{i,j+1,k} &= \frac{N}{S_4} \cdot \frac{\mathbf{F}_m}{\delta l^3}
\end{align*}
\]

\[
\frac{N}{S_1} + \frac{N}{S_2} + \frac{N}{S_3} + \frac{N}{S_4} = 1
\]
3. Fully resolved fluid-particle interaction: CFD

Mapping can formally be written as:

Euler $\rightarrow$ Lagrange:

$$\tilde{u}_m = \sum_{ijk} D(r_{ijk} - r_m) \cdot \tilde{u}_{ijk}$$

Lagrange $\rightarrow$ Euler:

$$\tilde{f}_{ijk} = \sum_m D(r_{ijk} - r_m) \cdot \frac{F_m}{\delta l^3}$$

mapping is of course not restricted to volume-weighing
Solution procedure to calculate variables at time $n+1$ including IBM force $f$:

1. **Initial guess:**
   \[ \hat{P}_{ijk}^{n+1} \Rightarrow \nabla \hat{P}_{ijk}^{n+1} \]

2. **Calculate velocity field without forcing**:
   \[ \tilde{u}_{ijk}^{n+1} = u_{ijk}^n - \frac{\delta t}{\rho} \nabla \hat{P}_{ijk}^{n+1} - \frac{\delta t}{\rho} A_{ijk}^n \]

3. **Map velocity field to marker point locations**:
   \[ \tilde{u}_m = \sum_{ijk} D(r_{ijk} - r_m) \cdot \tilde{u}_{ijk}^{n+1} \]

4. **Calculate IBM force at marker point locations**:
   \[ F_m = C \delta l^3 \cdot \frac{\rho}{\delta t} (w_m - \tilde{u}_m) \]

5. **Map IBM force to Eulerian grid**:
   \[ f_{ijk} = \sum_m D(r_{ijk} - r_m) \cdot F_m / \delta l^3 \]

6. **Calculate updated velocity field**:
   \[ \tilde{u}_{ijk}^{n+1} = u_{ijk}^n - \frac{\delta t}{\rho} \nabla \hat{P}_{ijk}^{n+1} - \frac{\delta t}{\rho} A_{ijk}^n + \frac{\delta t}{\rho} f_{ijk} \]

7. **Calculate pressure**:
   \[ \nabla \cdot \tilde{u}_{ijk}^{n+1} = \frac{\delta t}{\rho} \nabla^2 \Phi \]

8. **Update pressure**:
   \[ P_{ijk}^{n+1} = \hat{P}_{ijk}^{n+1} + \Phi \]

9. **Final update of velocity**:
   \[ u_{ijk}^{n+1} = \tilde{u}_{ijk}^{n+1} + \frac{\delta t}{\rho} \nabla \Phi \]
Initial guess:
\[
\tilde{P}_{ijk}^{n+1} \Rightarrow \nabla \tilde{P}_{ijk}^{n+1}
\]
\[
\tilde{u}_{ijk}^{n+1} \Leftarrow \nabla \tilde{P}_{ijk}^{n+1}
\]
\[
\tilde{u}_m \Leftarrow \tilde{u}_{ijk}^{n+1}
\]
\[
F_m = K (w_m - \tilde{u}_m)
\]
\[
f_{ijk} \Leftarrow F_m
\]
\[
\tilde{u}_{ijk}^{n+1} \Leftarrow f_{ijk}
\]
\[
\nabla \cdot \tilde{u}_{ijk}^{n+1} = \frac{\delta t}{\rho} \nabla^2 \Phi
\]

Solid phase:
\[
R_a(t), V_a(t)
\]
\[
r_m \text{ on surface of } a
\]
\[
w_m \forall m \in a
\]
\[
F_{f,a} = - \sum_{m \in a} F_m
\]
\[
F_{coll}^{ab}
\]
\[
M \dot{R}_a = \sum_b F_{coll}^{ab} + F_{f,a}
\]
\[
R_a(t + \delta t), V_a(t + \delta t)
\]

Output: drag correlation $F$

\[
\Phi
\]
\[
P_{ijk}^{n+1} = \tilde{P}_{ijk}^{n+1} + \Phi
\]
\[
u_{ijk}^{n+1} = \tilde{u}_{ijk}^{n+1} + \frac{\delta t}{\rho} \nabla \Phi
\]
First test: comparison with the exact expression by Hasimoto for a dilute SQ infinite array:

\[ F = \frac{F_{f,a}}{3\pi \mu d(u - V_a)} \]

\[ F_{\text{exact}} = \frac{1 - \phi}{1 - 1.7601\phi^{1/3} + \phi - 1.5593\phi^2} \]

\[ Fo = \nu \frac{\delta t}{\delta l^2} \]
3. Fully resolved fluid-particle interaction: CFD

Idea:
Use Hasimoto for setting an effective hydrodynamic diameter (calibration)

Note that also in LBM an effective diameter is used!

\[
F_{\text{exact}} = \frac{1 - \phi}{1 - 1.7601\phi^{1/3} + \phi - 1.5593\phi^2}
\]
3. Fully resolved fluid-particle interaction: CFD

Validation: drag for a dense square array:

\[ F = \text{Function of} \phi \text{ with diameter correction} \]
3. Fully resolved fluid-particle interaction: CFD vs LBM

Comparison with LB results for the drag for a dense random array:

\[ F(\phi) = \frac{F_{f,p}}{3\pi \mu u} = \frac{10\phi}{(1-\phi)^2} + \frac{1+1.5\phi^{1/2}}{(1-\phi)^{-2}} \]
3. Validation: Interaction force between 2 spheres
- Particles fixed at their position
- Particles have equal, but opposite velocities, with Re << 1
- Surface-to-surface distance s varied
- Results compared with exact solution from multipole expansion of the Stokes eq.
3. Validation: Interaction force between 2 spheres

3. Fully resolved fluid-particle interaction: CFD vs LBM

Thesis S.H.L. Kriebitzsch (2011)
Interaction force between two particles in relative motion

\[ \frac{d_o}{\delta l} = 9 \]

\[ \frac{d_o}{\delta l} = 17 \]

Thesis S.H.L. Kriebitzsch (2011)
3. Fully resolved fluid-particle interaction: CFD vs LBM

Interaction force between two particles in relative motion

\[ \frac{d_o}{\delta l} = 9 \]

\[ \frac{d_o}{\delta l} = 17 \]

Thesis S.H.L. Kriebitzsch (2011)
Three basic models for two-phase granular flow:

- DNS
- DEM
- TFM
II. DEM models for granular two-phase flow

\[ \mathbf{F}_{f,a} \text{ follows from stick boundary conditions} \]

\[ \mathbf{F}_{f,a} \text{ estimated from relations based on the local } \phi \]
Unresolved flow: implementation similar to resolved flow

\[ F_a = -F_{f,a} \]

\[ = 3\pi \mu (v_a - u_a) F(\phi) \]

\[ \frac{10\phi}{(1-\phi)^2} + \frac{1+1.5 \phi^{1/2}}{(1-\phi)^{-2}} \]

\[ F_m = C \delta l^3 \cdot \frac{\rho}{\delta t} (w_m - \bar{u}_m) \]
**Unresolved flow**: implementation similar to **resolved flow**

Note that $F(\phi)$ is the same for all particles that occupy the same cell.

To evaluate $\mathbf{u}_a$, again a Euler-Lagrange mapping is required.

\[
F_a = -F_{f,a} = 3\pi \mu (\mathbf{v}_a - \mathbf{u}_a) F(\phi)
\]

\[
= \frac{10\phi}{(1-\phi)^2} + \frac{1+1.5\phi^{1/2}}{(1-\phi)^{-2}}
\]
Initial guess:

\[ \hat{P}^{n+1}_{ijk} \Rightarrow \nabla \hat{P}^{n+1}_{ijk} \]

\[ \tilde{u}^{n+1}_{ijk} \Leftarrow \nabla \hat{P}^{n+1}_{ijk} \]

\[ \tilde{u}_m \Leftarrow \tilde{u}^{n+1}_{ijk} \]

\[ F_m = K \left( w_m - \tilde{u}_m \right) \]

\[ f_{ijk} \Leftarrow F_m \]

\[ \hat{u}^{n+1}_{ijk} \Leftarrow f_{ijk} \]

\[ \nabla \cdot \hat{u}^{n+1}_{ijk} = \frac{\delta t}{\rho} \nabla^2 \Phi \]

Solid phase:

\[ R_a(t), V_a(t) \]

\[ r_m \text{ on surface of } a \]

\[ w_m \quad \forall m \in a \]

\[ F_{f,a} = - \sum_{m \in a} F_m \]

\[ M \dot{R}_a = \sum_b F_{coll.}^{ab} + F_{f,a} \]

\[ R_a(t + \delta t), V_a(t + \delta t) \]

Output: drag correlation \( F \)

\[ P^{n+1}_{ijk} = \hat{P}^{n+1}_{ijk} + \Phi \]

\[ u^{n+1}_{ijk} = \hat{u}^{n+1}_{ijk} + \frac{\delta t}{\rho} \nabla \Phi \]
Initial guess:

\[ \hat{P}_{ijk}^{n+1} \Rightarrow \nabla \hat{P}_{ijk}^{n+1} \]

\[ \tilde{u}_{ijk}^{n+1} \Leftarrow \nabla \hat{P}_{ijk}^{n+1} \]

\[ \tilde{u}_a \Leftarrow \tilde{u}_{ijk}^{n+1} \]

\[ F_a = 3\pi \mu d \left( V_a - \tilde{u}_a \right) \cdot F \]

\[ f_{ijk} \Leftarrow F_a \]

\[ \tilde{u}_{ijk}^{n+1} \Leftarrow f_{ijk} \]

\[ \nabla \cdot \tilde{u}_{ijk}^{n+1} = \frac{\delta t}{\rho} \nabla^2 \Phi \]

Note: there are other implementations where velocity can be treated fully implicit.

Solid phase:

\[ R_a(t), V_a(t) \]

Input: drag correlation \( F \)

\[ F_{f,a} = -F_a \]

\[ F_{ab}^{\text{coll.}} \]

\[ M\dot{R}_a = \sum_b F_{ab}^{\text{coll.}} + F_{f,a} \]

\[ R_a(t + \delta t), V_a(t + \delta t) \]

\[ P_{ijk}^{n+1} = \hat{P}_{ijk}^{n+1} + \Phi \]

\[ u_{ijk}^{n+1} = \tilde{u}_{ijk}^{n+1} + \frac{\delta t}{\rho} \nabla \Phi \]
DEM models for granular two-phase flow

Comparison DEM/DNS

Deviation $\Delta F$ of true force from DP force
DEM models for granular two-phase flow

Comparison DEM/DNS

1. DEM drag is 33% lower than the average true drag force.
2. For 1 out of every 3 of the particles the individual force for deviates more than 25% with the DEM force.
DEM models for granular two-phase flow

Idea: use individual volume fractions $\phi_i$

$$\vec{F}_{g,i} = 3\pi \mu d (\vec{u} - \vec{v}_i) \cdot F(\phi_i, \text{Re})$$
DEM models for granular two-phase flow

Drag correlations derived for static system are not applicable to moving particles.

Natural spreading in the fluid-particle drag is too large to capture with (advanced) drag models in DEM.

Discrete element models are useful for obtaining insight, but should not be used for qualitative results.
III. Example: Effect of air on vibrated granular beds
Equal-sized bronze and glass spheres (100 µm)

Experiments by Burtally, King and Swift (Science 2002)

Simulations:

- Particles: “molecular dynamics” with soft-sphere model
- Gas phase: computational fluid dynamics model
- Gas-Particle interactions: unresolved, empirical drag force
- System size: \( N_p = 25\,000, \ W \times H \times D = 8 \times 6 \times 0.6 \, mm^3 \)
- Parameters: \( f = 55 \, Hz, \ A = 1 \, mm \quad \Rightarrow \quad \Gamma = \frac{A(2\pi f)^2}{g} = 12 \)

No air  

Air
Vibrated glass-bronze beds

Burtally, King, Swift & Leaper, Gran. Mat. 2003

\[ f = 55 \text{ Hz} \]
\[ A = 0.07 \text{ mm} \]
Vibrated glass-bronze beds

Experimental phase diagram (Burtally et al)

\[ \Gamma = \frac{A(2\pi f)^2}{g} \quad [\text{[-]}] \]

- \( f = 125 \text{ Hz} \)
- \( \Gamma = 9 \)

- Bronze on top
- Sandwich
Why do the light particles sink to the bottom?
Vibrated glass-bronze beds

Sandwich formation:

- Convection plays an important role
- Sensitive of the particle-particle and particle wall friction

<table>
<thead>
<tr>
<th>$\mu_{pp}$ ↓ $\mu_{pw}$ →</th>
<th>0.0</th>
<th>0.1</th>
<th>0.4</th>
</tr>
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<tbody>
<tr>
<td>0.0</td>
<td>Bottom</td>
<td>Bottom</td>
<td>Bottom</td>
</tr>
<tr>
<td>0.1</td>
<td>Middle (40 s)</td>
<td><strong>Middle</strong> (10 s)</td>
<td>Top</td>
</tr>
<tr>
<td>0.4</td>
<td>Middle (20 s)</td>
<td>Middle (10 s)</td>
<td>Top</td>
</tr>
</tbody>
</table>
Concluding remarks

DEM simulations are a “cheap” way to incorporate the effect of air, however, they should only be used for getting qualitative insight.

Almost all DNS simulations suffer from (large) grid resolution effects. The use of an effective diameter is essential for getting accurate results.
Key features of the model:

- Particles: soft-sphere model, 0.5 mm diameter
- Gas phase: computational fluid dynamics model
- Gas-Particle interactions: unresolved, empirical drag
- System size: $N_p = 14\,000$, $W \times H \times D = 100 \times 50 \times 2.1\, \text{mm}^3$
- Parameters: $f = 6.25\, \text{Hz}$, $A = 10\, \text{mm}$  \[ \Gamma = \frac{A(2\pi f)^2}{g} = 1.6 \]

With: Devaraj van der Meer
Ko van der Weele
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First documented by Da Vinci (1500) and Faraday (1831)
Mechanism for steady state heap