Simulation of granular flow in a fluid applied to sedimentation

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Abstract. We present a numerical model applied to the simulation of granular flow in a fluid. The description of particle flow is discrete. Particle trajectories are calculated by Newton’s law and collisions are described by a soft-sphere approach. The fluid flow is modelled using the Navier-Stokes equation. The momentum transfer is directly calculated from the stress tensor around particles. This model is validated through the calculation of the drag coefficient, making it possible to discern the limitations on the Reynolds number according to the mesh size and the computational time. The accuracy of the Navier-Stokes solver is estimated by the calculation of the hydrodynamic drag of a fluid flowing through a porous media at low Reynolds numbers. The analysis shows that dense media require a smaller mesh size than dilute media. This model is then used to describe the sedimentation of two particles to reproduce the "Draft, Kiss and Tumbled" effect. This shows the capacity of the model to reproduce hydrodynamic interactions acting on the scale of the particle. The terminal velocity of particles is in good agreement with experiments. Simulations of the sedimentation of a system of particles makes it possible to recover the Richardson and Zaki law in an acceptable CPU time.

1 Introduction

Several industrial processes use fixed beds, fluidized beds, pneumatic transport or sedimentation (see Fig. 1). Their correct operation requires the understanding of the behavior of a granular bed interacting with a fluid. However, the hydrodynamics of such processes is still badly known, bringing into play physical phenomena that act on the scale of the particle.

Numerical simulation is a tool which makes it possible to understand these phenomena. Several models can be used to simulate two phase flows of fluid-solid type:

1. Continuous models for the phases liquid and solid [1], [2], [3], [4], [5] are popular in the engineering sciences. In these models, questions remain open concerning the determination of the proper constitutive equation for the solid and the modelling of the momentum transfer between the solid and fluid phases. In general, the momentum transfer is modelled by a local drag force depending on the local relative velocity between the solid and the fluid, the Reynolds number and the local volume fraction of the solid and the fluid. This drag law is based on Ergun’s law [6] giving the pressure drop in a granular media.

2. Eulerian-Lagrangian models for the fluid and solid phases respectively [7], [8], [9], [10] implemented using a finite element method and no-slip boundary conditions on the surface of each particle have been employed for rather few particles. Recently, however, these methods

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have also been successful even to describe technological
problems, see e.g. [11]. The most accurate solvers for
the fluid phase use the finite element techniques where
a local refinement can be adapted to the particle sur-
face and to the local structure of the flow. This tech-
nique can reproduce very precisely the behavior, but
the remapping due to the particle motions is computa-
tionally expensive and a few particles can be simulated
in two dimensions.

3. Eulerian models for the fluid phase coupled to a dis-
crete description of the solid phase. [12], [13], [14], [15],
[16], [17], [18], [19] use a drag law. The main draw-
back of a drag law method is that a neglect of the proper
boundary conditions in the treatment of the
fluid will result in an inaccurate rendering of the short
scale flow properties. The boundary conditions on the
particle surface and their influence on the flow is then
represented by a point particle approximation with an
empirical or theoretical momentum exchange term.

4. The most powerful method in term of computational
effort, is the use of a fixed nonadaptive grid to represent
the fluid flow:
- [20] apply the lattice Boltzmann method and an
  extension to particle suspensions as introduced by
  Ladd et al. [21], [22].
- [23] propose an immersed boundary technique fol-
  lowing an idea of Fogelson and Peskin [24]
- [25], [26] integrate the stress tensor around the sur-
  face of the particles. Recently, this method has been
  successfully applied also to oblate shaped particles
  [27], [28].

In this paper, a model of type 4. is presented: The par-
ticle flow is discrete. Particle trajectories are calculated
through Newton’s law and collisions are described by a
soft-sphere approach. The fluid flow is calculated using
the Navier-Stokes equation solved on a staggered grid. The
momentum transfer is directly calculated from the stress
tensor around each particle.

2 Model

2.1 Particle flow

The dimensionless variables are obtained by dividing the
average particle radius \( r \) for the length, the Stokes ve-
locity \( V_s \) for the velocity and the fluid density \( \rho_f \). The
description of particle flow is discrete [29], [30], [31]. Par-
ticle trajectories are calculated through non-dimensional
Newton’s law and collisions are described by a soft-sphere
approach as follows:

\[
f_g + f_{ho} + f_h + f_n + f_t = m_{ip} \frac{d^2x_{ip}}{dt^2} \quad (i_p = 1, \ldots, n_p)
\]  

(1)

where \( m_{ip} \) is the mass of the particle \( i_p \) given by:

\[
m_{ip} = \frac{4}{3}\pi r_p^3 \rho_p \rho_f
\]  

(2)

The gravity force \( f_g \) is given by:

\[
f_g = -m_{ip} Fr u_{xip}
\]  

where the Froude number is given by:

\[
Fr = \frac{r g}{V_s^2}
\]  

(4)

The hydrostatic force \( f_{ho} \) is given by:

\[
f_{ho} = \frac{4}{3}\pi r_p^3 Fr u_{xip}
\]  

(5)

The momentum exchange between fluid and particulate
phase is done by the hydrodynamic force \( f_h \) will be dis-

cussed in section 2.3.

As the particles may collide during the simulations, we
introduce a central repulsive and dissipative force acting
if particles are in contact, described in the next section
2.1.1.

2.1.1 Collision forces

We describe the collision force in the normal direction by:

\[
f_n = f_{el} + f_{dn}
\]  

(6)

and in the tangential direction by the Coulomb law as fol-

\[
f_t = -\min(\mu_c ||f_n||, ||f_{dt} + f_s||) t
\]  

(7)

where \( \mu_c \) is the Coulomb friction coefficient.

The elastic restoring force \( f_{el} \) is given by:

\[
f_{el} = -k_n ([r_{ip} + r_{jp}] - \delta r) n
\]  

(8)

where \( n \) is the unit normal vector pointing from the center
of particle \( i \) to the center of particle \( j \):

\[
n = \frac{x_{ip} - x_{jp}}{||x_{ip} - x_{jp}||}
\]  

(9)

and

\[
\delta r = (x_{ip} - x_{jp}) \cdot n
\]  

(10)

The dissipative character of the contact is taken into ac-

\[
f_{dn} = -2 \gamma n m r c d v_n
\]  

(11)

where \( \gamma_n \) is the normal dynamic friction coefficient and
the normal velocity \( v_n \) is given by:

\[
v_n = ([v_{ip} - v_{jp}] \cdot n) n
\]  

(12)

in the tangential direction by \( f_{dt} \):

\[
f_{dt} = -2 \gamma t m r c d v_t
\]  

(13)
with the tangential velocity \( v_t \):

\[
v_t = v_{i_p} - v_{n}\tag{14}
\]

and by a static friction force \( f_s \) given by:

\[
f_s = -k_s \int_0^{t_c} v_t \, dt \tag{15}
\]

\( x_{i_p}, m_{i_p}, n_p, k_s, t_c, n_{i_p}, r_{e_p} \) and \( r_{f_p} \) are respectively the position, the mass of the particle \( i_p \), the total number of particles, the static friction coefficient, the collision time, the elastic modulus and the radius of particle \( i_p \) and \( j_p \).

\( m_{red} \) is the reduced mass given by:

\[
m_{red} = \frac{m_{i_p} m_{j_p}}{m_{i_p} + m_{j_p}} \tag{16}
\]

The integration of the equations of motion is carried out by using the explicit leap-frog scheme given in appendix A.1 with a time steps \( \Delta t_p \) for particle update given by:

\[
\Delta t_p = \frac{t_c}{25} << t_c \tag{17}
\]

where \( t_c \) is the collision time of two particles (see Fig. 2).

### 2.1.2 Linked-Cell algorithm

We use a linked list technique to reduce the \( O(n_p^2) \) operations required by the direct calculation of the interaction force. For considering only nearest neighbor possible collisions, the linked list technique takes only \( O(n_p) \) operations.

The shape of the simulation box is chosen to be a rectangular parallelepiped with dimensions \( L_x, L_y, L_z \), for simplicity. The simulation box is divided into \( N_{x_p} \times N_{y_p} \times N_{z_p} \) identical small cells of size two times larger than the maximum radius of the particles.

A particle in a given cell then only interacts with particles in the same or neighboring cells.

In the link list technique we construct a header array \( \text{header} \), which points, for each cell, to the first particle in that cell or to zero if the cell is empty. We construct the linked list array \( \text{link} \) as follow: to each particle indexed by \( 1, \ldots, n_p \), we assign a pointer, which points to the next particle in the same cell. The linked list ends, when the pointer of a particle is zero. The resulting algorithm is:

\[
\text{for } i = 1, N_{x_p} \\
\text{for } j = 1, N_{x_p} \\
\quad \text{header}(i, j, k) = 0 \\
\text{end for} \\
\text{end for} \\
\text{for } i_p = 0, n_p \\
\quad \text{link}(i_p) = 0 \\
\text{end for} \\
\text{for } i_p = 0, n_p \\
\quad i = \text{int}(N_{x_p} \times x_{i_p}/L_x) + 1 \\
\quad j = \text{int}(N_{y_p} \times y_{i_p}/L_y) + 1 \\
\quad k = \text{int}(N_{z_p} \times z_{i_p}/L_z) + 1 \\
\quad \text{link}(i_p) = \text{header}(i, j, k) \\
\quad \text{header}(i, j, k) = i_p \\
\text{end for}
\]

In the case of the Fig. 3, the algorithm gives:

\[
\text{header}[2][3] = 2, \text{link}[2] = 0 \\
\text{header}[4][3] = 4, \text{link}[4] = 11, \text{link}[11] = 0 \\
\text{header}[5][5] = 3, \text{link}[3] = 8, \text{link}[8] = 9, \text{link}[9] = 0
\]

The calculation of the interaction forces is done cell by cell using the \( \text{header} \) and the \( \text{link} \) arrays. Because of Newton's third law, only the lower neighbors cells need to be checked (see Fig. 4). The cost of the algorithm for the calculation of the interaction forces is of the order \( 13n_p n_c \), where \( n_c \) is the average number of particles in the cells. This algorithm goes like \( O(n_p^2) \) and has the advantage of well lending itself to parallelisation [30], [32].

The linked-cell algorithm is well described in Ref. [33].

### 2.2 Fluid flow

The fluid is considered incompressible and Newtonian. The dimensionless variables are obtained by dividing the
average particle radius $r$ for the length, the Stokes velocity $V_s$ for the velocity and the fluid density $\rho_f$. The non-dimensional Navier-Stokes equations describe the motion of the interstitial fluid with a resolution scale $h$ smaller than the particle size as shown by Fig. 5:

$$\frac{\partial v_i}{\partial t} = \frac{\partial(v_{ij}v_j)}{\partial x_j} - \frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 v_i}{\partial x_i^2} \quad (18)$$

and the conservation of the fluid mass gives with the incompressibility:

$$\frac{\partial v_i}{\partial x_i} = 0 \quad (19)$$

where the Reynolds number is defined as:

$$Re = \frac{\rho_f V_s r}{\mu_f} \quad (20)$$

As described in Ref.[34], we will not consider the time independent gravity contribution explicitly, but cancel it against the hydrostatic pressure and omit both terms from Eq.(18). The corresponding buoyancy forces will be taken into account explicitly in the equations of motion (1) by the hydrostatic force $f_{ho}$.

2.2.1
Numerical scheme

An explicit operator splitting, fractional-time-step method, first order in time proposed by Chorin [35] is used in the following to solve the Navier-Stokes equation:

$$\frac{v_i^{n+1} - v_i^n}{\Delta t_f} = - \frac{\partial p^{n+1}}{\partial x_i} - \frac{\partial (v_j^{n} v_j^{n})}{\partial x_j} + \frac{1}{Re} \Delta (v_i^{n}) \quad (21)$$

where $p^{n+1} = p(t_{n+1}, x_1, x_2, x_3)$ is the fluid pressure at the timestep $t_{n+1} = (n+1) \Delta t_f$ and $v_i^{n} = v_i(t_{n+1}, x_1, x_2, x_3)$ is the fluid velocity in the $x_i$ space direction at the timestep $t_n = (n) \Delta t_f$.

The introduction of the quantity $v_i^{n+\frac{1}{2}}$ as follow:

$$\frac{v_i^{n+1} - v_i^n}{\Delta t_f} = \frac{(v_i^{n+1} - v_i^{n+\frac{1}{2}}) - (v_i^{n} - v_i^{n+\frac{1}{2}})}{\Delta t_f} \quad (22)$$

gives:

$$\frac{v_i^{n+\frac{1}{2}} - v_i^n}{\Delta t_f} = - \frac{\partial (v_j^{n} v_j^{n})}{\partial x_j} + \frac{1}{Re} \Delta (v_i^{n}) \quad (23)$$

and

$$\frac{v_i^{n+1} - v_i^{n+\frac{1}{2}}}{\Delta t_f} = \frac{\partial p^{n+1}}{\partial x_i} \quad (24)$$

Taking the divergence of equation (24) gives a Poisson equation for the pressure:

$$\frac{\partial^2 p^{n+1}}{\partial x_j \partial x_j} = \frac{1}{\Delta t_f} \frac{v_i^{n+\frac{1}{2}}}{\partial x_i} \quad (25)$$

A staggered marker and cell (MAC) mesh as base for a second order spatial finite difference centered discretization is used to discretize each term [36]. The discrete Poisson equation for the pressure is given in appendix A.2, and is solved using the conjugate gradient method [37].

The time step $\Delta t_f$ for the fluid update is given by the stability condition [35]:

$$\Delta t_f = \min \left( \frac{h^2 Re}{6}, \frac{2}{\max(||v||^2) Re} \right) \quad (26)$$

2.3
Momentum transfer: the particle-fluid coupling

The hydrodynamic force acting on a body immersed in a fluid can be described by a surface integral of the stress tensor:

$$\sigma_{ij} = -p \delta_{ij} + \frac{1}{Re} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \quad (27)$$

So, the momentum transfer between the fluid and the particle is directly calculated and obtained from the hydrodynamic force $f_h$ given by:

$$(f_h)_i = \int_{S_p} \sigma_{ij} n_j dS_p \quad (28)$$

where $S_p$ refers to the surface of the particle $i_p$ and $n_j$ is
the normal vector to the surface of the particle.

Numerically, we compute the force acting on the particles by decomposing the particle surface into square patches perpendicular to the coordinate axes.

As visualized in Fig. 6, the discrete expression for the stress tensor $\sigma_{ij}$ is calculated on each patch, multiplied by the normal vector $n_j$ and the area $h_j^2$ of each patch and then summed over all surface patches. The discrete expression for the stress tensor $\sigma_{ij}$ is given in Appendix A.3.

### 2.4 Computational time

The CPU time is about $6\mu s$ per node and per time step on a Silicon Graphics Workstation Octane with a R10000 processor.

The CPU time goes like $O(R^3)$, where $R$ is the reduction ratio of the mesh size with:

- $O(R^2)$ for the stability condition (26)
- $O(R^3)$ for the number of nodes.

For example, when a smaller mesh size $h_3 = 0.2r$ is used instead of $h_1 = 0.4r$, the reduction ratio is $R = 2$ and the CPU time is multiplied by $R^3 = 32$.

Large Reynolds numbers require a smaller mesh size given by the relation:

$$\frac{h}{r} = O(Re^{-\frac{9}{2}})$$

and consume too much CPU time.

### 3 Drag law

#### 3.1 Empirical expression of the drag law

The drag coefficient $C_d$ on a spherical particle of radius $r$ fixed in a fluid flow is defined by:

$$C_d = \frac{f_h}{2\rho_f U_s^2}$$

$f_h$ is the norm of the hydrodynamic force acting on the spherical particle, $U_s$ is the norm of the superficial fluid velocity and $\rho_f = \pi r^2$ is the cross section of the particle. The drag coefficient is a function of the Reynolds number.

The drag force can be determined analytically only for special cases. For a single rigid spherical particle moving in an infinite fluid with relative velocity $v_r$, at low Reynolds number $Re' \ll 1$, the insertion of the Stokes drag force:

$$f_h = 6\pi r \mu_f v_r$$

in the definition of the drag coefficient (30) gives the following drag coefficient:

$$C_d = \frac{24}{Re'}$$

with: $Re' = \frac{2r \rho_f v_r}{\mu_f}$

For particle Reynolds numbers higher than unity the drag coefficient must be determined from experiments. With increasing Reynolds number the contribution of the form drag becomes more important and finally dominates over the viscous drag. In the range $750 < Re' < 3 \times 10^5$ the drag coefficient approaches a nearly constant value of $C_d = 0.44$. This is known as inertial regime.

A reasonably good approximation for the drag coefficient of spherical particles in the transitional region between the Stokes and inertial regime, $0.2 < Re' < 1000$, is the correlation of Schiller and Naumann [38]:

$$C_d = \frac{24}{Re'}(1 + 0.15Re'^{0.487})$$

#### 3.2 Parameters and boundary conditions

Fig. 7 illustrates the simulation box and the dimensions are: $L_x = 20r$, $L_y = 40r$ and $L_z = 20r$. We see no change of the results using a bigger box (relative error less than 1%).

The particle is placed at the position (see Fig. 7.):

$$x_p = (\frac{L_x}{2}, \frac{L_y}{4}, \frac{L_z}{2}).$$

The particle positions and orientations are fixed during each time step of the simulation. The simulations are performed as dynamical calculations starting from a fluid field at rest until a steady flow state results.

We choose two different mesh sizes: $h_1 = 0.4r$ and $h_2 = 0.2r$ at a moderate Reynolds number. The time step is calculated from the stability condition (26).
We used as boundary conditions an uniform non-dimensional velocity \( U_s = 1.0 \) on \( x_2 = 0 \), a pressure set to zero on \( x_2 = L_{x_2} \) and periodic boundary conditions on \( x_1 \) and \( x_3 \) space direction. 

3.3 Results

Fig. 8 shows the drag coefficient calculated by the simulation as a function of the Reynolds number \( Re' \).

Expression (33) for the drag coefficient for \( Re' \leq 20 \) is reproduced with a maximal error of 14% with a mesh size of \( h_1 = 0.4r \) and a maximal error of 10% with a mesh size of \( h_2 = 0.2r \).

So, the simulation is in fair agreement with the empirical law of Schiller and Nauman for \( Re' \leq 20 \). Larger Reynolds numbers require a smaller mesh size and consume too much computer time (see 2.4).

4 Hydrodynamic drag of fluid flow through a porous media

To estimate the accuracy of the fluid flow model, we consider a fluid flowing through a porous media at low Reynolds numbers. The porous media is a cubic periodic arrangement of fixed spheres. The simulation results are compared with the Sangani analytical expression, the Ladd numerical results and the empirical Ergun’s law.

Fig. 8. Drag coefficient as a function of the Reynolds number \( Re' \).

4.1 Expressions of the hydrodynamic drag

The hydrodynamic non-dimensional drag force \( K \) on a spherical particle of radius \( r \) is defined by:

\[
K = \frac{f_h}{6\pi r} \frac{U_s}{U_f}
\]  

where \( f_h \) is the modulus of the hydrodynamic force, \( \mu_f \) is the fluid viscosity and \( U_s \) is the superficial fluid velocity.

In the limit of infinite dilution, the determination of the hydrodynamic drag is equivalent to the case of a single spherical particle falling in a medium at rest at infinity. The insertion of the Stokes drag force in Eq. (34) gives \( K = 1 \).

For moderate volumic concentration of solid and low Reynolds numbers, Sangani [39] have found with a point particle approximation the following analytic expression of the hydrodynamic drag force as function of volumic concentration of solid \( \Phi \):

\[
K^{-1} = 1 - 1.7601\Phi^2 + 1.5593\Phi^2 + 3.9799\Phi^2 - 3.0734\Phi^2 + O(\Phi^2)
\]

Among others, Ladd [40] as well as Sangani and Acrides have considered larger volumic concentrations of solid up to the limit of \( \Phi_m = \frac{\pi}{6} \) with numerical methods in the Stokes approximation.

On another side, for the volumic concentration of solid \( \Phi \) to the limit \( \Phi_m = \frac{\pi}{6} \), the localized form of the empirical
Ergun law used by Tanaka et al [18] leads to the following hydrodynamic force:

\[ f_h = \frac{\pi \mu l}{3(1 - \Phi)^2} (150 \Phi + 1.75 Re) v_r \]  
(36)

where \( v_r \) is the relative velocity between the fluid and the particle.

Replacing the hydrodynamic force (36) in the definition of the hydrodynamic drag (34), and using:

\[ \|v_r\| = (1 - \Phi) U_s \]  
(37)

gives the corresponding hydrodynamic drag \( K \) for \( Re << 1 \) and \( \Phi_m = \frac{\pi}{6} \):

\[ K = \frac{25 \Phi_m}{3 (1 - \Phi_m)^3} \]  
(38)

4.2 Parameters and boundary conditions

Fig. 9 illustrates the simulation box and the dimensions are: \( L_{x1} = 10r, L_{x2} = 20r \) and \( L_{x3} = 10r \).

We see no change of the results using a bigger box (relative error less than 1%).

The particles positions and orientations are fixed during each time step of the simulation. The simulations are performed as dynamical calculations starting from a fluid field at rest until a steady flow state results.

We choose different mesh sizes: \( h_1 = 0.4r, h_2 = 0.2r, h_3 = 0.1r, h_4 = 0.05r \) and Reynolds number \( Re = 0.01 \). The simulations are done with \( n_p = 1 \) to \( n_p = 125 \).

The time step is calculated from the stability condition (26).

We used as boundary conditions an uniform non-dimensional velocity \( U_s = 1 \) on \( x_2 = 0 \) and on \( x_2 = L_{x2} \) and periodic boundary conditions on \( x_1 \) and \( x_3 \) space direction.

4.3 Results

To find the accuracy of the method, we measure the error defined by Eq. (39) as a function of the mesh size of the hydrodynamic drag with a volume concentration of solid \( \Phi = \frac{\pi}{6} \) and \( Re = 0.01 \):

\[ error = \frac{|f_h \text{ calculated } - f_h \text{ Ladd}|}{\max(f_h \text{ calculated } , f_h \text{ Ladd})} \times 100 \]  
(39)

Fig. 10 shows that the accuracy of the method leading error proportional to the mesh size \( h \) due to the approximation of the particle surface.

Fig. 11. shows the calculated hydrodynamic as a function of volumic concentration of solid \( \Phi \) and Fig. 12 illustrates a snapshot of the velocity field.

We see a satisfactory agreement of the calculated hydrodynamic drag with previous results of other authors leading error below 1% with a mesh size of \( h_4 = 0.05 \). These simulations show the limitations due to the mesh size: direct simulations in a diluted medium \( \Phi < 0.1 \) can be carried out with a grid of mesh size \( h_1 = 0.4r \) and the higher volumic concentrations with a smaller mesh size of \( h_4 = 0.05 \).

The reason for these limitations comes from the fact that the denser the medium, the smaller are the pores through which the fluid can pass requiring a finer resolution.

5 Draft, Kiss and Tumbled Effect

The model is used to simulate the sedimentation of two particles and to reproduce the Draft, Kiss and Tumbled effect.
the hydrodynamic drag above particle 2. As the hydrodynamic drag of particle 2 is a depression zone, particle 1 is attracted inside. The Draft.Particle 1 increases its vertical velocity until it touches particle 2. The Kiss. The horizontal velocity of particle 2 increases and its vertical velocity decreases below that of particle 1. Particle 1 having the same horizontal velocity and higher vertical velocity than particle 2, overtakes particle 2; the Tumbled.

5.2 Parameters and boundary conditions
We use the following physical parameters:
\[ \rho_f = 1000 \text{kg.m}^{-3}, \rho_p = 2000 \text{kg.m}^{-3}, \mu_f = 10^{-3} \text{kg.s.m}^{-1}, r = 100 \mu m \]
giving the three non-dimensional parameters:
\[ Re = \frac{\mu_f V_s}{\rho_f} = 2.2 \]
\[ St = \frac{2 \rho_p V_s}{\rho_f} \frac{\mu_f}{9} = 0.97 \]
\[ Fr = \frac{\rho_f g}{\rho_f V_s^2} = 2.1 \]
where: \( V_s = \frac{2 \rho_f (\rho_p - \rho_f)}{9 \mu_f} \)

We use gravity in the \( x_2 \) space direction.
The particle 1 is placed at the initial position:
\[ x_p = (\frac{L_{x_1}}{2}, \frac{L_{x_2}}{4}, \frac{L_{x_3}}{4}) \]
and the particle 2 at the initial position:
\[ x_p = (\frac{L_{x_1}}{2}, \frac{L_{x_2}}{4}, \frac{L_{x_3}}{4}) \]
The initial velocity of the particles is null.
The mesh size is \( h = 0.4r \) and the stability condition gives the time step \( \Delta t_f = 5.8 \times 10^{-2} \). The dimensions of the simulation box are:
\[ L_{x_1} = 12r, L_{x_2} = 24r \text{ and } L_{x_3} = 12r \]
We use periodic boundary conditions for velocity and pressure of the fluid in each space direction.

5.3 Results
The simulation reproduces the Draft, Kiss and Tumbled effect of the sedimentation of two particles under gravity. Fig. 13 and Fig. 14 show the pressure fields and the velocity of the fluid at \( x_3 = \frac{L_{x_3}}{2} \) at times \( t = 14 \) corresponding to the Draft. Fig. 13 shows the depression zone corresponding on negatives values of fluid pressure behind the particle 2 in agreement with the experimental description of the Draft.

Fig.15, Fig. 16, Fig. 17 show respectively the velocity of the fluid at \( x_3 = \frac{L_{x_3}}{2} \) at times \( t = 77 \) corresponding to the Draft, just before the Kiss, at times \( t = 88 \) corresponding to the Kiss and at times \( t = 126 \) corresponding to the Tumbled.
Fig. 13. Pressure fields of the fluid at $x_3 = \frac{L_{x3}}{2}$ at times $t = 14$ corresponding to the Draft.

Fig. 14. Velocity fields of the fluid at $x_3 = \frac{L_{x3}}{2}$ at times $t = 14$ corresponding to the Draft.

Fig. 15. Velocity fields of the fluid at $x_3 = \frac{L_{x3}}{2}$ at times $t = 77$ corresponding to the Draft, just before the Kiss.

Fig. 16. Velocity fields of the fluid at $x_3 = \frac{L_{x3}}{2}$ at times $t = 88$ corresponding to the Kiss.

6 Sedimentation of a system of particles

6.1 The empirical law of Richardson and Zaki

The mean velocity $\bar{v}$ of a system of particles sedimenting in a fluid depends on the volumic concentration of the solid $\Phi$ through the Richardson and Zaki [41] law:

$$\bar{v}(\Phi) = V_s (1 - \Phi)^n$$  \hspace{1cm} (40)

where $V_s$ is the Stokes velocity of an isolated particle.

The exponent $n$ is a function of the Reynolds number and is close to 5 for Reynolds numbers $Re \leq 1$. This law
is confirmed by many experiments and in particular by Nicolai et al. [42].

6.2 Parameters

We use the following physical parameters: $\rho_f = 1000 \text{kg.m}^{-3}$, $\rho_p = 2500 \text{kg.m}^{-3}$, $\mu_f = 10^{-3} \text{kg.s.m}^{-1}$, $r = 50 \mu m$

giving:

$Re = 0.41$, $Fr = 7.4$ and $St = 0.23$ and a non-dimensional time step of $\Delta t_f = 10^{-2}$.

We use gravity in the $x_2$ space direction.

The simulations are done with $n_p = 1$ to $n_p = 12500$.

Fig. 20 illustrates the simulation box and the initial particle positions. The dimensions are:

$L_{x_1} = 40r$, $L_{x_2} = 80r$ and $L_{x_3} = 40r$. Periodic boundary conditions are used in each space direction.
6.3 Results

The simulations carried out for mesh sizes $h_1 = 0.4r$ and $h_2 = 0.2r$ yield the law (40) for different volume concentrations $\phi$ (see Fig. 21). These simulations show the limitations due to the mesh size: direct simulations in a diluted medium can be carried out with a grid of mesh size $h_1 = 0.4r$ and volume concentrations $\phi$ below 0.2 with $h_2 = 0.2r$. As explain in 4, the reason for these limitations comes from the fact that the denser the medium, the smaller are the pores through which the fluid can pass requiring a finer resolution.

Fig. 22 and Fig. 23 illustrate respectively the pressure and the velocity field of the flow in the region defined by $x_3 = \frac{L_{x_3}}{2}$ and $0 \leq x_2 \leq \frac{L_{x_2}}{2}$. The depression zone corresponds on negatives values of fluid pressure shown by Fig. 22.

We see the change of particle locations and particle numbers (53 compared to 60) in regard to the initial setup given by Fig. 20 due to the hydrodynamic interactions.

7 Conclusions

We presented a model to simulate granular flow in a fluid. A discrete method is used for the granular medium, where the trajectories of the particles are calculated using Newton’s law with a soft sphere approach. The flow of the fluid is determined solving the Navier-Stokes equations on a fixed grid with a small mesh size compared to the size of the radius of the particles. The momentum transfer between the fluid and the solid phases is carried out directly integrating the stress tensor over the surface of each particle.

This method is sufficiently accurate to reproduce hydrodynamic drag of a fluid flowing through a porous media at low Reynolds numbers. The analysis shows that dense media require a smaller mesh size than diluted media.

The simulation of the sedimentation of two particles reproduces the Draft, Kiss and Tumbled effect in good agreement with experiments. This shows the capacity of the model to calculate hydrodynamic interactions acting on the scale of the particle.

Simulations of the sedimentation of a system of many particles reproduces the law of Richardson and Zaki with the same conclusions: Dense media impose smaller mesh sizes than dilute media. The method requires an accept-
able computing time and makes it possible to treat on a workstation of the order of one thousand particles in three dimensions. Larger Reynolds' numbers cannot be simulated with this method since they lead to prohibitory computing times. Summarizing, this model can be used to describe and validate local transfers between the solid and fluid phases. It is possible to use implicit numerical techniques to overcome some of the apparent limitations, in particular the need for very short time steps with a fine mesh size.

8 Acknowledgments
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A Appendix
A.1 Numerical scheme
The integration of the equations of motion is carried out by using the explicit leap-frog scheme derived by writing the following Taylor expansion:

\[ v_{i_{p}}^{n+\frac{1}{2}} = v_{i_{p}}^{n} + \frac{\Delta t_{p}}{2} a_{i_{p}}^{n} + \frac{\Delta t_{p}^{2}}{4} \frac{d^{2} v_{i_{p}}}{dt^{2}} + O(\Delta t_{p}^{3}) \] (41)

\[ v_{i_{p}}^{n-\frac{1}{2}} = v_{i_{p}}^{n} - \frac{\Delta t_{p}}{2} a_{i_{p}}^{n} + \frac{\Delta t_{p}^{2}}{4} \frac{d^{2} v_{i_{p}}}{dt^{2}} + O(\Delta t_{p}^{3}) \] (42)

\[ x_{i_{p}}^{n+1} = x_{i_{p}}^{n} + \Delta t_{p} v_{i_{p}}^{n} + \frac{\Delta t_{p}^{2}}{2} a_{i_{p}}^{n} + O(\Delta t_{p}^{3}) \] (43)

with:

\[ x_{i_{p}}^{n} = x_{i_{p}}(n\Delta t_{p}) \quad v_{i_{p}}^{n} = v_{i_{p}}(n\Delta t_{p}) \quad f_{tot_{i_{p}}}^{n} = f_{tot_{i_{p}}}(n\Delta t_{p}) \]

and leads to the following algorithm:

1. The velocity at time step \((n + \frac{1}{2})\Delta t_{p}\), obtained by subtracting Eq. (42) from Eq. (41), is calculated by:

\[ v_{i_{p}}^{n+\frac{1}{2}} = v_{i_{p}}^{n-\frac{1}{2}} + \Delta t_{p} a_{i_{p}}^{n} \] (44)

with:

\[ a_{i_{p}}^{n} = \frac{f_{tot_{i_{p}}}^{n}}{m_{i_{p}}} \] (45)

2. The position at time step \((n + 1)\Delta t_{p}\), obtained by Eq.(43) is calculated by:

\[ x_{i_{p}}^{n+1} = x_{i_{p}}^{n} + \Delta t_{p} v_{i_{p}}^{n+\frac{1}{2}} \] (46)

A.2 Discrete Poisson equation for the pressure
A staggered marker and cell (MAC) mesh (see Fig. 24) as base for a second order spatial finite difference centered discretization is used to discretize each term [36] with:

\[ v_{p_{i}}(n+\frac{1}{2}) = v_{1}(k + \frac{1}{2}l, m) \quad x_{p_{i}}(n+\frac{1}{2}) = v_{2}(k, l + \frac{1}{2}m) \quad \text{• corresponds to the pressure } p \text{ at the node } (k, l, m). \]

The discrete Poisson equation for the pressure is given by:

\[ \frac{1}{h^{2}}(p_{i}^{n+1} - p_{i}^{n-1} + p_{i}^{n+1} - p_{i}^{n-1} + p_{i}^{n+1} - p_{i}^{n-1} + p_{i}^{n+1} - p_{i}^{n-1} - 6p_{i}^{n+1}) = \]

\[ \frac{1}{h^{2}}(v_{i}^{n+\frac{1}{2}} - v_{i}^{n-\frac{1}{2}} + \frac{\Delta t_{p}}{2} a_{i_{p}}^{n}) \]

\[ \frac{1}{h} \left[ \frac{n+\frac{1}{2}}{h} + \frac{n-\frac{1}{2}}{h} \right] \]

\[ + v_{i}^{n+\frac{1}{2}} \left[ \frac{n+\frac{1}{2}}{h} - \frac{n-\frac{1}{2}}{h} \right] \]

\[ + v_{i}^{n-\frac{1}{2}} \left[ \frac{n+\frac{1}{2}}{h} - \frac{n-\frac{1}{2}}{h} \right] \]

\[ \frac{1}{h^{2}}(v_{i}^{n+\frac{1}{2}} - v_{i}^{n-\frac{1}{2}} + \frac{\Delta t_{p}}{2} a_{i_{p}}^{n}) \] (47)

The discretization produces external nodes, like: \(v_{1}(\frac{1}{2}, \frac{1}{2}, m)\) and \(v_{2}(\frac{1}{2}, \frac{1}{2}, m)\).

The velocity value at this node is determined through a linear extrapolation.

For example at the node \((-\frac{1}{2}, \frac{1}{2}, m)\), we have:

\[ v_{2}(-\frac{1}{2}, \frac{1}{2}, m) = 2v_{2} + 2v_{1}(\frac{1}{2}, \frac{1}{2}, m) \] (48)

To fix the value of \(v_{1}(\frac{1}{2}, \frac{1}{2}, m)\), we write:

\[ v_{1}(\frac{1}{2}, \frac{1}{2}, m) = v_{1}(\frac{1}{2}, \frac{1}{2}, m) \] (49)

The boundary condition for the pressure is determined by calculating the scalar product of the discretized equation.
(4) with the normal unit vector of the domain boundary:

\[
\frac{p^{n+1}_{i,j,k,m} - p^{n+1}_{-i,-j,k,m}}{h} = -\frac{1}{\Delta t} \left( v^{n+\frac{1}{2}}_{i+\frac{1}{2},-j,k,m} - v^{n+\frac{1}{2}}_{i,-j+\frac{1}{2},k,m} \right)
\]

Replacing Eq. (50) in Eq. (47), the quantity \( v^{n+\frac{1}{2}}_{i+\frac{1}{2},-j-k,m} \) is cancelled and gives for the boundary node:

\[
v^{n+\frac{1}{2}}_{i+\frac{1}{2},-j-k,m} = v^{n+\frac{1}{2}}_{i,-j-k,m} \text{ (51)}
\]

\[
p^{n+1}_{i,-j,k,m} = p^{n+1}_{i+1,j,k,m} \text{ (52)}
\]

The Poisson equation (47) for the pressure with the boundary condition (52) is solved using the conjugate gradient method [37].

A.3

Discrete expression of the stress tensor

By using the staggered marker and cell (MAC) mesh, the discrete expression for the stress tensor \( \sigma_{ij} \) is given by:

\[
(f_{k})_{i} = \kappa^{2} \sum_{(k,j,m)} -p_{(k,l,m)}\eta_{i} + \frac{1}{Re} \frac{1}{h} \sigma_{ij} \eta_{j} \text{ (53)}
\]

with:

\[
\sigma_{11} = 2(v_{k+\frac{1}{2},j,k,m} - v_{k-\frac{1}{2},j,k,m})
\]

\[
\sigma_{22} = 2(v_{k,j+\frac{1}{2},k,m} - v_{k,j-\frac{1}{2},k,m})
\]

\[
\sigma_{33} = 2(v_{k,j,k+\frac{1}{2},m} - v_{k,j,k-\frac{1}{2},m})
\]

\[
\sigma_{12} = v_{k+\frac{1}{2},j+\frac{1}{2},k,m} - v_{k-\frac{1}{2},j-\frac{1}{2},k,m} + v_{k+\frac{1}{2},j-\frac{1}{2},k,m} - v_{k-\frac{1}{2},j+\frac{1}{2},k,m}
\]

\[
\sigma_{13} = v_{k+\frac{1}{2},j,k+\frac{1}{2},m} - v_{k-\frac{1}{2},j,k-\frac{1}{2},m} + v_{k+\frac{1}{2},j,k-\frac{1}{2},m} - v_{k-\frac{1}{2},j,k+\frac{1}{2},m}
\]

\[
\sigma_{23} = v_{k,j+\frac{1}{2},k+\frac{1}{2},m} - v_{k,j,k-\frac{1}{2},m} + v_{k,j,k+\frac{1}{2},m} - v_{k,j,k-\frac{1}{2},m}
\]

\[
\sigma_{31} = v_{k+\frac{1}{2},j,k+\frac{1}{2},m} - v_{k-\frac{1}{2},j,k-\frac{1}{2},m} + v_{k+\frac{1}{2},j,k-\frac{1}{2},m} - v_{k-\frac{1}{2},j,k+\frac{1}{2},m}
\]

Notation

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r )</td>
<td>non-dimensional average radius of particle</td>
</tr>
<tr>
<td>( n_{p} )</td>
<td>number of particles</td>
</tr>
<tr>
<td>( m_{p} )</td>
<td>mass of particle</td>
</tr>
<tr>
<td>( \eta_{i} )</td>
<td>non-dimensional tangential friction coefficient</td>
</tr>
<tr>
<td>( \eta_{n} )</td>
<td>non-dimensional normal friction coefficient</td>
</tr>
<tr>
<td>( \mu_{s} )</td>
<td>Coulomb friction coefficient</td>
</tr>
<tr>
<td>( \rho_{p} )</td>
<td>solid density</td>
</tr>
<tr>
<td>( \rho_{f} )</td>
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<tr>
<td>( C_{D} )</td>
<td>drag coefficient</td>
</tr>
<tr>
<td>( K )</td>
<td>non-dimensional hydrodynamic drag</td>
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<tr>
<td>( \Phi )</td>
<td>volumetric solid concentration</td>
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<tr>
<td>( \tau_{ij} )</td>
<td>non-dimensional stress tensor</td>
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<tr>
<td>( Re )</td>
<td>Reynolds number</td>
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<td>( St )</td>
<td>Stokes number</td>
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<tr>
<td>( Fr )</td>
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