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Assessment of a coupled VOF-Front-Tracking/DEM method for simulating fluid-particles flows

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Abstract

In this paper we introduce a one-fluid numerical method for the simulation of dense particle-fluid flows. The method uses a front tracking algorithm coupled to a viscous penalty method to enforce the rigidity constraint. A modified version of the collision model of Mohaghegh and Udaykumar (2019) is used to model both collisions and lubrication forces. This approach allows us to greatly reduce the amount of ad hoc numerical parameters required to perform the simulations. For validation purpose, we successfully reproduce several experimental and numerical benchmarks including the settling case of a sphere in an enclosed box performed by ten Cate et al. (2002), the bouncing motion against a planar surface performed by Gondret et al. (2002), the study of the fluid-solid fluidized bed performed by Aguilar-Corona (2008), and the particle-resolved simulations of the same case performed by Ozel et al. (2017). The method is shown to realistically reproduce the motion of a settling and a bouncing sphere in a quiescent fluid. The statistical study of the fluidized bed showed excellent agreement with the experimental data and the fluidization law: the solid volume fraction, the solid velocity variance and the anisotropy coefficient are accurately reproduced by our simulations.

Keywords: Particulate flows, Fluidized bed, Front-Traking, One-fluid method, Discrete Element Method, Soft Sphere Model.

1. Introduction

Fluid-particles systems are of considerable scientific and technological interest in a wide range of disciplines. They can be encountered in environmental flows as for example in sandstorms, river sediment transport or dispersal of volcanic ashes to cite just a few. In engineering, one can find them for example in pneumatic transport, pollution control or fluidized beds. The latter are ubiquitous in the chemical and energy fields because of their excellent mixing properties. Since 2010, an original concept of high temperature solar receivers using solid-gas fluidized bed as heat transfer fluid is being actively developed at the CNRS (France) Flamant and Hemati (2010); Flamant et al. (2013); Benoit et al. (2015); Zhang et al. (2017); Gueguen et al. (2021). Indeed, the heat transfer fluids currently used in tower

power plants (*i.e.* molten salts) limit the temperature at the receiver outlet below 560°C. In the framework of the third generation of receivers development, the trend is to increase the receiver outlet temperature in order to use high efficiency thermodynamic cycles downstream (super-critical cycle). For this purpose, the target temperature at the receiver outlet is 800°C. Fluidized bed appears to be an excellent heat transfer fluid candidate.

The literature on the experimental studies of fluidization phenomena is extensive. Often, flat, pseudo-two-dimensional fluidized beds are used to investigate the fluidization behavior with the aid of video techniques or probe measurements because three-dimensional fluidized beds are not optically accessible (Müller et al. (2008)). The main limitation of such experimental techniques is that the probes locally disturb the fluidization behavior and thereby affect the measurement itself. To address these restrictions, detailed computational models have received substantial attention over the last thirty years. With the use of computer models,

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one can realize non-intrusive numerical experiments to examine the flow-field. Furthermore, the use of appropriate models enables the simultaneous ‘measurement’ of several properties, such as the gas and particle velocities, and the porosity, which is difficult if not impossible to achieve by direct experimentation. Despite these advantages, the construction of reliable models for large-scale gas–solid systems is seriously hindered by the lack of understanding of the fundamentals of dense gas–particle flows. The prime difficulty here relies on the large separation of scales (Ge et al. (2017)): the largest flow structures can be of the order of meters; yet these structures are directly influenced by the details of particles–particles and fluid-particles interactions, which take place on the scale of millimeters, or even micrometers

In this context various frameworks have been developed, i.e Two-Fluid Model (TFM), Discrete element method (DEM), Direct numerical simulations (DNS), each one of them targeting a particular level of precision or scale (see Sundaresan et al. (2018) for a comparative review of these methods). One can then use the smaller scale models to develop closure laws for the larger scale models. Recently, thanks to the continuous increase in computing power, studying large particle-laden flows with finite-size particles using particle-resolved direct numerical simulations (DNS) has become possible. In the past few decades, many researchers have used particle-resolved simulations to gain a deeper understanding of the intricate physics behind flow-particle and particle-particle interactions in a variety of configurations. These simulations have been applied in a range of fields, including fluidized beds Pan et al. (2002); Ozel et al. (2017); Esteghamatian et al. (2017); Yao et al. (2021), sedimentation Uhlmann (2005); Uhlmann and Doychev (2014); Willen and Prosperetti (2019), particles induced/interaction with turbulence Uhlmann (2008); Lucci et al. (2010); Wang et al. (2014); Picano et al. (2015); Fornari et al. (2016); Costa et al. (2016), and sediment patterns in channel flow Kidanemariam and Uhlmann (2017) among others.

Generally speaking, in the DNS approach, the governing equations for the fluid phase and the particles are implicitly coupled with each other through the no-slip condition at the particles’ surfaces (2-way coupling) without the need for parametrizing the drag force between the phases. Also, long-range hydrodynamic interactions between particles are naturally captured. However, when dense flows are considered (flows with particles close enough to directly interact), additional models are required to account for short-range solid-fluid interactions (lubrication forces) and solid-solid contacts

(collisions forces). The common approach to model a wet collision is to use a spring-damper system for the solid dissipation, and the lubrication theory for the viscous dissipation.

The goal of this paper is to present an extension of the Front-Tracking method of the simulation software TrioCFD (Calvin, Christophe et al. (2002)) to include solid–solid contact forces by means of a soft-sphere model, and to assess its capability for simulating particle-fluid flow. The resulting algorithm allows for the reduction of the number of numerical parameters required for the simulations. The Front-tracking aspect allows for a precise description of solid-fluid interfaces, which will be extremely useful when studying collisions between non-spherical particles in a future study. More specifically, we developed a method that uses Lagrangian markers to describe the solid-fluid interface. The method is developed for flows with particles of any shape. Obviously, in the tested configurations where only spherical particles are considered this method is not optimal. Indeed, we use several hundreds of Lagrangian markers to describe the surface of one sphere whereas only two parameters - the gravity center and the radius - are required. However, in the case of particles of arbitrary shape, a Lagrangian surface mesh of the solid-fluid interface become a significant asset to accurately describe the interface. To the best of the authors’ knowledge, there is no combination of front-tracking approach and viscous penalty method in the literature.

We first start by presenting in section 2 the Front-Tracking method along with the soft-sphere model used for the solid–solid contact forces. This coupled DNS–DEM technique is then validated in Section 3 through simulations of various validation cases from the literature. In section 4, we perform simulations of fluidized bed, and present a comparison of the simulation results against numerical and experimental data obtained by Ozel et al. (2017) and Aguilar-Corona (2008). This test serves to validate the coupled DNS–DEM approach in a case with many particles simultaneously interacting. Finally, in section 5 we draw some concluding remarks concerning this study and prospects for future work.

2. Governing equations and numerical method

The algorithm used in this work to perform direct numerical simulations of fluid-particles flow is based on the “one-fluid” formalism. In this approach, a single set of equations is used to describe the behavior of all

phases present in the computational domain. The different phases are treated as a single fluid with spatially varying material properties, depending on the phase indicator function. The governing equations are given by:

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0 \\ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot (\mu (\nabla \mathbf{u} + \nabla^T \mathbf{u})) + \rho \mathbf{g} + \mathbf{F}_c \end{aligned} \quad (1)$$

Where $\mathbf{u}$ is the velocity field, ρ the density field, p the pressure field, μ the dynamic viscosity field, $\mathbf{g}$ the gravitational acceleration, and $\mathbf{F}_c$ the collisional force. Both phases are considered incompressible. ρ and μ are considered constant within each phase but show an abrupt transition across the interface. The equations are identical to the equations of a single-phase flow. Therefore, the techniques developed to solve the equations for single-phase flows can readily be used. The only difference is that the solver must be adapted to handle spatially varying material properties. Here we will use a staggered grid to solve the previous equations (Fig. 1 – Right). When solving numerically equations (1), it is necessary to identify which phase is present at a given location. To do this, a phase indicator function I is introduced. It is set to 1 in the solid phase, 0 in the fluid phase and is equal to the solid volume fraction $\alpha = V_{solid}/V_{cell}$ in all the cells crossed by an interface (Fig 1). In two-phase cells, the density is defined as a mean of the fluid and the solid densities weighted by the phase indicator. Such arithmetic averaging allows to be consistent with the mass conservation principle:

$$\rho = I\rho_{solid} + (1 - I)\rho_{fluid} \quad (2)$$

The same averaging procedure cannot be used for the viscosity field, as it needs to satisfy a different kind of condition (Ritz and Caltagirone (1999)). The following subsection provides more information about this aspect.

As the particles move, the interface between the two phases is displaced. Being able to precisely locate the position of the interface is of paramount importance in the one-fluid formalism. The advection of the marker function is governed by:

$$\frac{\partial I}{\partial t} + \mathbf{u} \cdot \nabla I = 0 \quad (3)$$

Despite the apparent simplicity of the Eq. (3), the numerical integration of a discontinuous color function is one of the difficult problems in computational fluid dynamics. Over the years several methods such as the volume-of-fluid (VOF) method, The level-set method have emerged to address this problem (see Tryggvason

et al. (2011) for a review on the subject). In this work we will focus on one method in particular, i.e. the Front Tracking method (Bunner and Tryggvason (2003)).

2.1. General description of the Front-Traking method

According to this method, the boundary between the two phases is tracked by a moving surface mesh composed of connected Lagrangian marker points that are advected relatively to a fixed Eulerian mesh (Fig. 1 – Left). The flow equations are solved on the Eulerian fixed mesh. The interface velocity is calculated by first doing a tri-linear interpolation of the background velocities at each marker location (Fig. 1 – Right). The barycentric velocity of the interface $\dot{\mathbf{u}}_m$ is then numerically calculated from:

$$\dot{\mathbf{u}}_m = \frac{1}{\sum A_i} \sum A_i \dot{\mathbf{u}}_i \quad (4)$$

where A_i and $\dot{\mathbf{u}}_i$ are respectively the area, and the velocity vector associated to the i^{th} marker of the Lagrangian mesh. The markers are then translated with the barycentric velocity:

$$\dot{\mathbf{x}}_i^{n+1} = \dot{\mathbf{x}}_i^n + \Delta t \dot{\mathbf{u}}_m^{n+1} \quad (5)$$

Once the new positions of the markers $\dot{\mathbf{x}}_i^{n+1}$ are known, the front is used to reconstruct the indicator function and to update the local physical properties accordingly. The difficulties usually raised by the front tracking method, related to mass conservation and the management of fragmentation and coalescence of inclusions, are absent in our situation. Indeed, as we simulate only solid-fluid flows with perfectly rigid interfaces, there is no need to utilize the expensive remeshing procedures intended to correct the degradation of the interface as it deforms over time. The special treatment intended to enforce the rigidity constraint within the solid phase is described below.

2.2. Imposing the rigid body motion

In classical Lagrangian mechanics, an object without any internal degrees of freedom is referred to as a “rigid body”. Within such entity, the distance between two arbitrary points is always constant. Mathematically, for this condition to be fulfilled, it is necessary and sufficient for the velocity field inside the solid region to satisfy:

$$\mathbf{U}(\mathbf{X}) = \mathbf{U}_c + \boldsymbol{\omega} \times (\mathbf{X} - \mathbf{X}_c) \quad (6)$$

where $\mathbf{X}_c$ is the position of the center of mass, $\mathbf{U}_c$ is the velocity of the center of mass and $\boldsymbol{\omega}$ is the angular velocity of the rigid body motion. From an Eulerian point

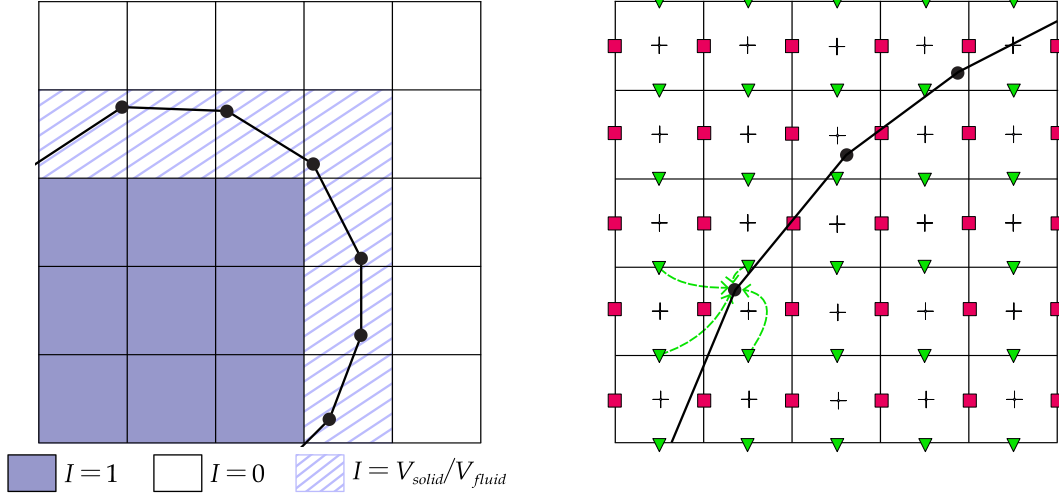


Figure 1: (Left) Schematic illustration of the phase Indicator function and the front-tracking approach. (Right) Interpolation of the y-component of the velocity at a marker position on a 2D staggered grid: the black crosses, pink squares and green triangles indicate respectively the pressure, x-component and y-component velocity calculation points, the black dots materialize the Lagrangian marker.

of view, this condition can be expressed as equating the strain rate to 0 (Temam and Miranville (2005)):

$$\frac{1}{2} (\nabla \mathbf{u} + \nabla^T \mathbf{u}) = \mathbf{0} \quad (7)$$

This formulation is of great convenience with regard to the "one-fluid" equations discussed previously. It describes a localized constraint for the rigid domain that could be directly imposed over the momentum conservation equation without the need to know the velocities of the solid beforehand. Practically, it is possible to nullify the deformation tensor by imposing a high value for μ inside the solid region relative to the fluid domain. The rigid body behavior will be in that case asymptotically enforced. Such an approach is called a viscous penalty method (Ritz and Caltagirone (1999); Caltagirone and Vincent (2001)). This strategy has the advantages to greatly simplify the coupling between the solid-fluid phases since the coupling is done implicitly and the inertia of the solid region is fully carried by the fluid solver. The velocity field inside the solid being a divergence-free field, the continuity equation is also automatically satisfied.

To impose solid body motion, a large value of the fictitious viscosity must be imposed in the solid region. This led to the existence of large viscosity ratios in the vicinity of the interface and especially in cells where the phase indicator function $I \in]0, 1[$, hereafter called diphasic flow cells. The calculation of the average viscosity in those cells is of great importance to properly

reproduced the friction force applied by the fluid flow on the particle. A possible way to compute the latter is to apply an arithmetic average, as it is done for the average density. Doing so will result in a negligible contribution of the fluid viscosity to the average regardless of the solid volume fraction. If $\mu_{solid} \gg \mu_{fluid}$ then:

$$\mu = I\mu_{solid} + (1 - I)\mu_{fluid} \approx I\mu_{solid} \quad (8)$$

This will have the negative effect of making the solid appear larger than it actually is. By propagating the penalty effects to the flow near the interface, the drag forces affecting the motion of the solid is therefore overestimated. As signaled by Ritz and Caltagirone (1999), using a harmonic average would better satisfy the condition of stress continuity at the interface. However, even with this strategy, the viscosity ratio can occasionally be so high that additional treatments are required. For example, some authors proposed to reduce the radius of the particles to compensate for this effect (Vincent et al. (2014); Thiam (2018)). For the numerical investigations conducted in this paper, it was shown that utilizing a step function to apply the fluid viscosity to both the fluid cells and the two-phase cells produced the best results. It should be noted that fine-tuning the viscosity ratio is necessary before starting the simulations, as imposing low viscosity inside the particle will lead to a poorly enforced rigidity constraint. In this study a viscosity ratio between 10^3 and 10^4 is taken.

2.3. Short-range interaction modeling

In general, Non-Boundary-Fitted-Particle-Resolved (NBF-PR) methods, such as the one discussed in the previous section, are ideally suited to capture the long-range hydrodynamic interactions between the fluid and solid phases. However, they are not the best suited methods to capture the short-range interactions. The lubrication effects are under resolved, and the collisions are not taken into account intrinsically by NBF-PR methods. Additional modeling is required to take those interactions into account.

2.3.1. Lubrication modeling.

As two solids are brought very close to one another, the fluid between the two surfaces is drained out of its location, generating viscous constraints. The NBF-PR methods performs a decent job of capturing the frictional forces as long as the distance between the two solids is greater than two simulation cells. In the case where the spacing becomes smaller than one cell, the viscous stress is in fact under resolved. A more realistic alternative would be to rely on a closure model based on the lubrication theory to make up for the grid's lack of spatial resolution (Cox and Brenner (1967); Cooley and O'Neill (1969)). In Breugem (2010), the author implemented this approach by adding an amplified Stokes drag force on the solid when the space between the solid surfaces dropped below a predetermined user-defined distance. This distance corresponds to the threshold under which the simulation method fails to solve the fluid dynamics accurately. To avoid the divergences of the analytical expression of the lubrication force, Breugem capped it starting from another user specified distance. Physically, it was justified as a means to simulate the saturation of the hydrodynamic force caused by roughness effects. As the force constantly opposes the particle's motion, it is a dissipative force by nature.

Several authors have successfully used this kind of closure procedure to model the viscous lubrication effects (Kempe and Fröhlich (2012); ten Cate et al. (2002); Costa et al. (2015); Ardekani et al. (2016); Biegert et al. (2017); Izard et al. (2014); Brändle de Motta et al. (2013)). However, this approach can be problematic in a number of ways: the lubrication model's implementation might result in a large number of ad hoc numerical parameters that must be calibrated. For instance, three separate parameters were required in Brändle de Motta et al. (2013). Additionally, the provided amplification coefficients for the lubrication force are grid dependent. Moreover, in Biegert et al. (2017) the authors showed that the dissipation may depend on the gap thickness,

and more investigation is needed in that regard. Finally, for this procedure to be valid, the Stokes flow assumption must be fulfilled within the fluid film separating the two solids. This is only verified if the distance between the two interfaces is significantly smaller than the characteristic length scale of the particles (Cox and Brenner (1967)). To correctly solve for viscous dissipation in the fluid film, the mesh would need to be further refined, at the expense of computation time.

2.3.2. Collision modeling

As the surfaces of the particles come into direct contact, a collision occurs and affect the momentum of both particles. Most of the time, the trajectories are abruptly altered. According to Legendre et al. (2006), regardless of whether the collision happens in air (dry collision) or in a more viscous fluid (wet collision), the typical collision period is often several orders of magnitude shorter than the particle's viscous relaxation time. As a result, the particles perceive the collision as a discontinuity in their motions. Fully capturing the motion of the particles as they undergo collisions will require incredibly short integration time steps that would make simulating a particulate flow over an extended period of time impossible. For that reason, many authors preferred to model the collisions using a variation of the soft-sphere collision model of Cundall and Strack (1979). In the latter, the contact force applied to colliding solids is proportional to the distance separating their contact points. Glowinski et al. (1999) used a repulsive force proportional to the square of the distance separating the particles. The force that models lubrication in liquid-fluidized bed is applied from a distance beyond the particle surface to prevent any overlapping. Wan and Turek (2006) used a similar approach but the particles were allowed to overlap. Although straightforward to implement, using such force results in poor physical fidelity. Since the collision is viewed as elastic, the energy dissipation during the collision is not taken into consideration.

Based on the Hertz theory of contacts (Hertz (1882); Johnson (1985)), other authors suggested computing a nonlinear contact force using a mass-spring-damper system Kempe and Fröhlich (2012).

The coefficients of the model are derived from geometrical properties and from the particle elastic characteristics. The solid dissipation can be addressed thanks to the dash-pot coefficient. This approach is well concordant with the dry collisions experiments in Stevens and Hrenya (2005). The order of the time step of the Navier-Stokes solver is larger than the collisions duration predicted by the Hertz contact theory. Due to this

separation of time scales, extremely small numerical integration time steps are needed to solve the particle motion. Fortunately, it is possible to artificially stretch the collision duration to be larger than the fluid solver time step and still maintain the perceived separation of time scales (or the discontinuity) in the motion of the particles. Based on this principle, [Feng et al. \(2010\)](#) manually reduced the value of the spring stiffness value to obtain a satisfactory collision time. [Kempe and Fröhlich \(2012\)](#) suggested in their adaptive collision model (ACM) to stretch the collisions time to ten times the flow solver time step. Similarly, to the Hertz theory, a non-linear force-displacement relationship was used to model the contact force. The spring and dash-pot coefficients were computed by solving a second-order ordinary differential equation using an iterative solver. [Ray et al. \(2015\)](#) improved on the work of Kempe and Fröhlich by proposing an explicit formulation for the coefficients, alleviating the need for an iterative solver. In a similar fashion, [Breugem \(2010\)](#); [Brändle de Motta et al. \(2013\)](#); [Izard et al. \(2014\)](#); [Costa et al. \(2015\)](#) used the work of [van der Hoef et al. \(2006\)](#) to model the collision force with a damped harmonic oscillator. Which can be seen as a linearized version of the work of Kempe and Fröhlich. The spring stiffness and the damping coefficient are computed from the prescribed collision time and coefficient of restitution in a more straightforward way. A common factor among the studies mentioned above is that they were paired with a lubrication model to account for the dissipative effect of the viscous drainage. Besides that, the rebound velocity is unknown beforehand, as it can only be determined after the collision has ended.

2.3.3. Combined modeling

With the Simplified Spring Collision Method (SSCM), [Mohaghegh and Udaykumar \(2019\)](#) developed a different strategy that simultaneously accounts for both the dissipative effect in the solid and in the fluid gap. The collision force is modeled based on a mass spring system with no dash-pot. Such methodology allows to reduce the number of numerical parameters introduced. The spring stiffness is chosen to satisfy the specified maximum distance of collision. This distance is the only numerical parameter of the model. No damping coefficient or lubrication model is employed in the SSCM. Instead, the spring stiffness is adjusted using the coefficient of restitution to obtain the appropriate rebound velocity. The adjustment is made during the bouncing phase, which occurs after the particle has stopped moving at the "maximum distance of collision" and has begun to rebound in the opposite direction

of the impact. The SSCM differs from other models in that the rebound velocity of the particles is known before the impact even occurs. This is so because, the coefficient of restitution used to correct the spring stiffness is calculated from a well-established experimental relationship between the restitution coefficient and the Stokes number [Ruiz-Angulo and Hunt \(2010\)](#). The SSCM addresses many of the drawbacks of the precedent collision models. It allows the collision time to be stretched, enabling granular flow simulations to be run for extended times. The model's coefficients are provided explicitly, eliminating the requirement for an iterative solution. The number of numerical parameters is reduced to one (the maximum distance of collision), since no separate lubrication model is used.

In this paper we use a slightly modified version of [Mohaghegh and Udaykumar \(2019\)](#), as there is a quite obvious equivalence between the maximum distance of collision and the collision duration, the latter was preferred to compute the spring stiffness coefficient. We discuss the details of our modifications in the following. Consider a collision occurring between two spherical particles p and q or between the particle p and a wall. The contact force $\mathbf{F}_c$ acting on a particle during a collision is modeled by a harmonic oscillator as:

$$\mathbf{F}_c = -k\delta_n\mathbf{n} \quad (9)$$

with k is the spring stiffness and δ_n the normal distance separating the colliding sphere surfaces given by:

$$\delta_n = \|\mathbf{x}_p - \mathbf{x}_q\| - (R_p + R_q) \quad (10)$$

where $\mathbf{x}_p$ and $\mathbf{x}_q$ are the positions of the center of mass of the particles p and q , R_p and R_q are the radius of the particles. $\mathbf{n}$ is the normal vector to the plan of collision defined by:

$$\mathbf{n} = \frac{\mathbf{x}_p - \mathbf{x}_q}{\|\mathbf{x}_p - \mathbf{x}_q\|} \quad (11)$$

The differential equation describing the motion of the system is given by:

$$m_e\ddot{\delta}_n + k\delta_n = 0 \quad (12)$$

The spring stiffness k was derived by [Breugem \(2010\)](#) in the special case of an elastic collision:

$$k = m_e \left(\frac{\pi}{\tau_0} \right)^2 \quad (13)$$

where m_e is the effective mass and τ_0 is the prescribed collision time. For particle-particle interactions, $m_e = m_p m_q / (m_p + m_q)$ with m_p and m_q being the mass of

particles p and q respectively. If the collision occurs between a particle p and a wall, then $m_e = m_p$. The stretched collision time is taken as a multiple N of the Navier-Stokes solver time step Δt :

$$\tau_0 = N\Delta t \quad (14)$$

Physically, collisions are inelastic, which means that some kinetic energy is dissipated during the contact. Even, in the scenario where the viscous stress is negligible, some energy is still dissipated as vibrations in the solid. The dry coefficient of restitution e_d accounts for this energy dissipation:

$$e_d = \frac{\Delta u_{reb,d}}{\Delta u_{imp,d}} \quad (15)$$

where $\Delta u_{reb,d}$ and $\Delta u_{imp,d}$ are, respectively, the rebound and impact relative velocities of the two solid surfaces colliding in the absence of fluid viscous dissipation (dry regime). The solid's dry coefficient of restitution is a physical property directly related to the material's elastic properties. The default value used in this work is $e_d = 0.97$.

In the wet regime, the energy dissipation is notably higher due to the fluid viscous dissipation. [Joseph et al. \(2001\)](#); [Yang and Hunt \(2006\)](#) have shown experimentally that the apparent or effective coefficient of restitution is strongly correlated with the Stokes number St :

$$St = \frac{2 R_{eff} \Delta u_{imp} \rho_s}{9 \mu_f} \quad (16)$$

where R_{eff} is the effective radius – defined by $R_{eff} = R_p R_q / (R_p + R_q)$ in the case of two particles, and $R_{eff} = R_p$ in the case of a wall-particle collision –, Δu_{imp} is the relative velocity at the moment of impact, ρ_s the density of the particles and μ_f the dynamic viscosity of the fluid.

The relationship between the effective coefficient of restitution e and the Stokes number St can be written as the product of the constant dry coefficient of restitution and a "wet" coefficient of restitution, e_w depending on the St number. Typically e_w varies from 0 to 1:

$$e(St) = e_d e_w(St) = \frac{\Delta u_{reb}}{\Delta u_{imp}} \quad (17)$$

From Fig 2, we can see the effective coefficient of restitution e is pretty much equal to the dry coefficient of restitution for $St > 1000$. This is in accordance with the fact that in this range of Stokes numbers, viscous effects are negligible. However, for lower values of St , from 10 to 1000, significant variation of e is observed. The coefficient of restitution decrease with St and the related

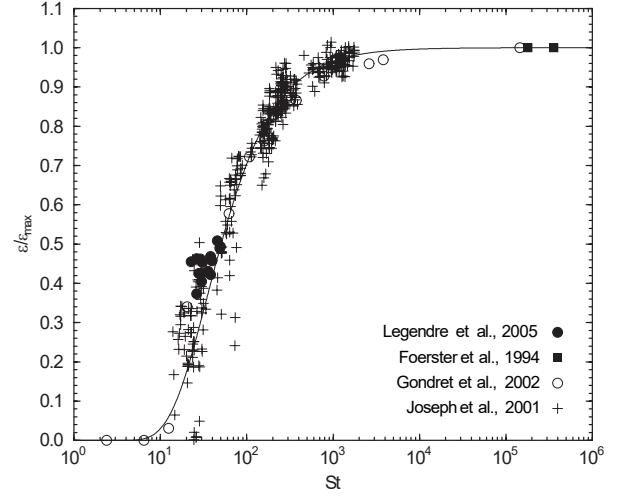


Figure 2: Adapted from [Legendre et al. \(2006\)](#). Wet coefficient of restitution, as a function of the Stokes number St . The solid line is the best fit of the data points of [Joseph et al. \(2001\)](#); [Gondret et al. \(2002\)](#); [Legendre et al. \(2005\)](#); [Foerster et al. \(1994\)](#)

viscous stress rise. Below the critical value St 10, no rebound is observed. Using the analogy with a dissipative mass-spring system [Legendre et al. \(2005\)](#) showed that the evolution of the wet coefficient of restitution as a function of the St numbers followed the expression:

$$e_w = \exp\left(-\frac{35}{St}\right) \quad (18)$$

Similarly to [Mohaghegh and Udaykumar \(2019\)](#), the required rebound velocity at the end of a collision is obtained by using the $e_w(St)$ relationship (Eq. 18) as an entry parameter of the model. The collision's effective coefficient of restitution is calculated based on the collision St number before impact and is used to adjust the spring stiffness in Eq. 9. Such procedure eliminates the requirement for a lubrication model or a dash-pot coefficient by intrinsically accounting for both energy dissipation. It is worth noticing that the pre-collision Stokes number is calculated at the time when the particles start to collide. This means that the lubrication effect has been already under-resolved, since the gap between the particles is less than a grid-cell. Hence, the Stokes number could be over-estimated. Practically speaking, the kinetic energy of the particle before and after the collision are prescribed using the effective coefficient of restitution. The difference between the two energies correspond to the dissipative effects. After translating this difference into potential energy, it can easily be shown that, to obtain the desired rebound velocity, the

spring stiffness needs to be reduced by a factor of e^2 in the rebound phase (see Mohaghegh and Udaykumar (2019) for more detail about the derivation). The adjustment is made after the maximum overlap of the interfaces allowed by the spring stiffness is reached, and the particles start to go in opposite ways. The spring stiffness is treated as piece-wise function of the scalar product $\Delta \mathbf{u} \cdot \mathbf{n}$ (Eq. 19). The change of sign of the latter is used to pinpoint the exact moment when the reduction of stiffness is done (see Fig 3):

$$k_i = \begin{cases} k_{imp} = m_e \left(\frac{\pi}{\tau_0} \right)^2 & \text{if } \Delta \mathbf{u} \cdot \mathbf{n} \leq 0 \\ k_{reb} = k_{imp} e^2 & \text{if } \Delta \mathbf{u} \cdot \mathbf{n} > 0 \end{cases} \quad (19)$$

The collision force $\mathbf{F}_c = -k_i \delta_n \mathbf{n}$ is then applied to the purely solid cells in the simulation domain (corresponding to Indicator function strictly equal to 0). This is done at each time step until there is no overlapping between the two solids.

2.4. Numerical implementation

The Navier–Stokes equations are solved by a prediction/correction method on a staggered Cartesian grid with a Marker-And-Cell finite volume discretization (MAC) Puckett et al. (1997). The velocity increment $\dot{\mathbf{u}}$ in the prediction step (Eq. 20) is calculated by summing the contributions of the convection term $\mathbf{A}^n$, the diffusion term $\mathbf{D}^{n+1}$, the collisional source term $\mathbf{C}^{n+1}$, and the gravitational source term $\mathbf{g}$. The pressure is not taken into account in this step:

$$\dot{\mathbf{u}} = \frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} = -\mathbf{A}^n + \frac{1}{\rho^n} (\mathbf{D}^{n+1} + \mathbf{C}^{n+1}) + \mathbf{g} \quad (20)$$

To alleviate the numerical constraints caused by the high viscosity ratios R_μ required by the viscous penalty method. The evaluation of the diffusive source term is implicit and computed with an Uzawa algorithm. Regarding the calculation of the collision term $\mathbf{C}^{n+1}$, the distance δ_n (Eq. 10) between the surfaces of each pair of particles p and q is calculated. If $(\delta_n < 0)$ then a collision is detected and the force to be applied to each of these particles is calculated. According to the third Newton law of motion, the reaction force to be applied to the particle q is of equal intensity and opposite direction to the force applied to the particle p :

$$\mathbf{F}_{c,p \rightarrow q} = -\mathbf{F}_{c,q \rightarrow p} \quad (21)$$

The forces acting on the particle p are summed up and divided by the volume V_p of the particle p . The result is

then applied to the appropriate solid cells thanks to the phase indicator function:

$$\mathbf{c}^{n+1} = I^n \sum_q \frac{\mathbf{F}_{c,q \rightarrow p}^{n+1}}{V_p} \quad (22)$$

The forces are calculated at each time step until no overlapping is observed ($\delta_n \geq 0$). The time integration of the collision force is done by a Semi Implicit Euler time scheme (SIE) to prevent numerical divergences caused by the Forward Euler scheme:

$$\mathbf{F}_{c,q \rightarrow p}^{n+1} = -k_i \delta_n^{n+1} \mathbf{n} \quad (23)$$

where $\mathbf{n}$ is given by Eq. 11 and δ_n^{n+1} is the distance separating the surface of the two colliding particles evaluated at the time $n + 1$:

$$\delta_n^{n+1} = \left\| (\mathbf{x}_p^n - \mathbf{x}_q^n) + \Delta t (\mathbf{u}_p^n - \mathbf{u}_q^n) \right\| - (R_p + R_q) \quad (24)$$

As the coefficient N (Eq. 14) is the only numerical parameter of our model, we discuss its influence in more detail in the following. The spring stiffness during the negative phase ($\Delta \mathbf{u} \cdot \mathbf{n} < 0$) is obtained by setting the collision duration $\tau_0 = N \Delta t$. However, when the spring stiffness is reduced in the positive phase ($\Delta \mathbf{u} \cdot \mathbf{n} > 0$), the collision period is stretched due to the oscillation period being inversely proportional to the spring stiffness. By noting that $T_{reb} = T_{imp}/e$ and:

$$\tau = \frac{1}{2} \left(\frac{T_{imp}}{2} + \frac{T_{reb}}{2} \right) \quad (25)$$

where T_{imp} and T_{reb} are the oscillation periods corresponding to the spring stiffness k_{imp} and k_{reb} , we can show that the stretching factor is equal to:

$$\frac{\tau}{\tau_0} = \frac{1}{2} \left(1 + \frac{1}{e} \right) \quad (26)$$

Fig. 4 (a) illustrates the evolution of the stretching factor as a function of N for various coefficients of restitution e . We can see that the initial collision duration τ_0 is retrieved in the dry regime (high Stokes numbers corresponding to $e = 1$). In the asymptotic case where $e \rightarrow 0$, the collision duration tends to infinity, and no rebound is observed as the particles remain in permanent contact.

Considering the relationship between N and the collision duration τ , it is important to keep N as small as possible to maintain physical realism at high Stokes numbers. However, N must be high enough for the collision force to be accurately integrated, as integration errors increase when N decreases. In order to demonstrate

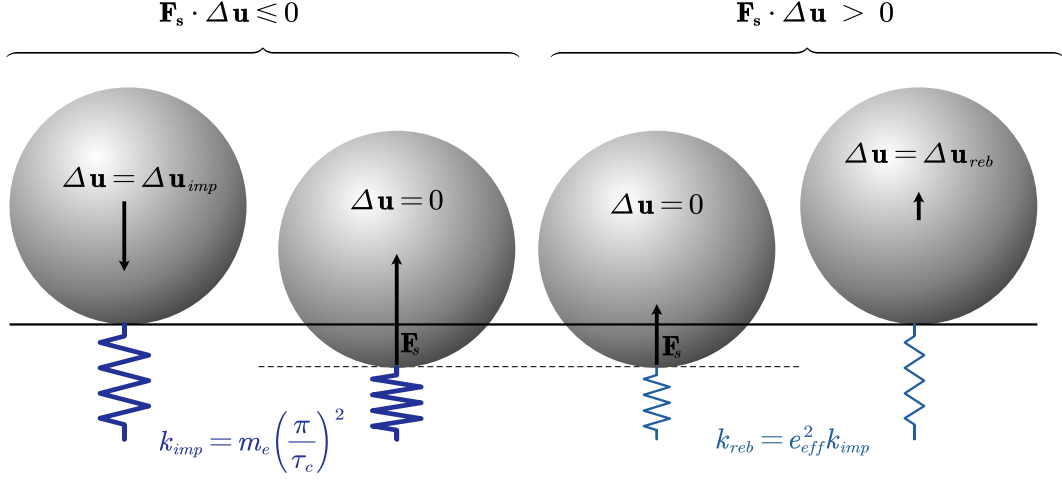


Figure 3: Explanatory diagram of the collision model.

this concept, we have numerically solved Eq. 12 using a semi-implicit Euler scheme. The spring stiffness of the system is defined by Eq. 19. Fig. 4 (b) illustrates the evolution of the integration error, which is defined as $|e_{err}| = |e - e(N)|/e$, where $e(N)$ represents the coefficient of restitution obtained after numerically solving Eq. 12 with an Euler Semi-Implicit method.

In our work, we have set $N = 8$ similarly to Breugem (2010); Brändle de Motta et al. (2013); Costa et al. (2015). For this value, the integration error in the dry regime is less than 1 percent. However, due to our model's nonlinear nature, the integration error increases as the coefficient of restitution decreases. For e equal to 0.65, 0.45, and 0.15, the integration error is equal to 0.038, 0.085, and 0.71, respectively. To reduce the integration error at lower Stokes numbers, N can be increased (see Fig. 4 (b)). However, this comes at the cost of losing physical realism at higher Stokes numbers. Alternatively, higher-order integration schemes can be used, but they come at the expense of computing time and memory consumption. In the collision validation section, we compared our simulation results to experimental data. We found that the overestimation of the rebound velocity introduced by the numerical integration scheme was negligible compared to the additional viscous damping effect exerted by the surrounding fluid. Therefore, we selected a value of $N = 8$ and the ESI scheme for the following simulations, as this choice was seen a good balance between computation time, accuracy, and physical realism.

In the case of a wall-particle collision, a virtual particle identical to the particle p is generated behind the wall as proposed in Glowinski et al. (1999). This strat-

egy allows the calculation of the collisions force in the wall-particle collisions situation to be treated in an identical manner to the particle-particle scenario. The virtual particle's center of mass is positioned so that the contact point is displaced from the wall by a distance ε_{wp} . Due to numerical restrictions unique to our simulation code, which prohibit Lagrangian points from leaving the simulation domain, the use of this offset is necessary. It was observed that this numerical limitation may be overcome with hardly any impact on the accuracy of the simulations provided in the next section by taking ε_{wp} equal to one fourth of the simulation grid cell.

Once the contributions corresponding to each source term in Eq. 20 is known, the predicted velocity field $\mathbf{u}^*$ is then obtained by using an Euler Explicit (EE) time scheme:

$$\mathbf{u}^* = \mathbf{u}^n + \dot{\mathbf{u}}\Delta t \quad (27)$$

Then, an elliptic pressure equation is solved by a SSOR-preconditioned GCP solver to impose a divergence-free velocity field:

$$\nabla \cdot \left(\frac{1}{\rho^n} \nabla P^{n+1} \right) = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}^* \quad (28)$$

From the resulting pressure field, we can compute the projected velocity field $\mathbf{u}^{n+1}$ by:

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \frac{1}{\Delta t} \nabla P^{n+1} \quad (29)$$

The freshly obtained Eulerian velocity field is used to compute the velocity $\dot{\mathbf{u}}_i$ at the position of Lagrangian nodes thanks to a tri-interpolation procedure $\mathcal{F}()$:

$$\dot{\mathbf{u}}_i^{n+1} = \mathcal{F}(\dot{\mathbf{x}}_i^n, \mathbf{u}^{n+1}) \quad (30)$$

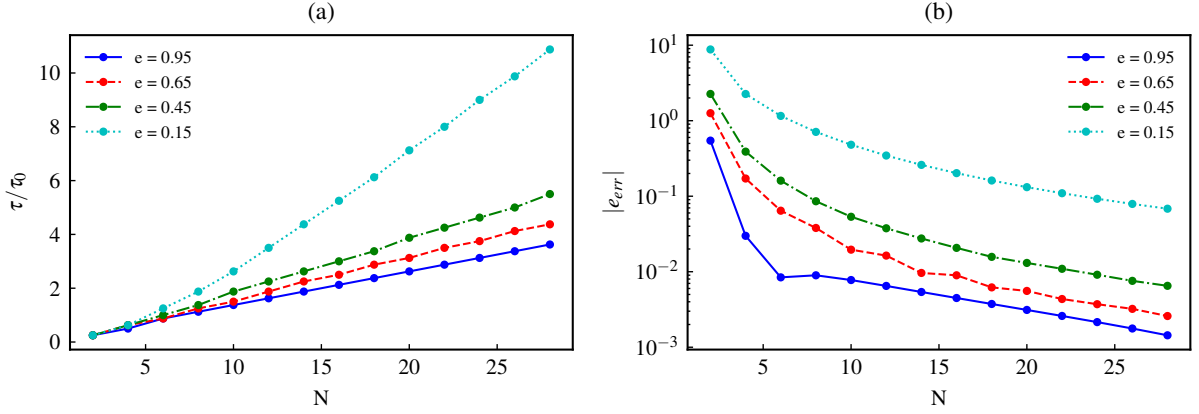


Figure 4: (a) Evolution of the collision duration stretching factor as a function of N for different coefficients of restitution e . (b) Evolution of the integration error as a function of N for different coefficients of restitution e .

The velocities of the Lagrangian nodes are used to compute a mean velocity of the interface $\hat{\mathbf{u}}_m$:

$$\hat{\mathbf{u}}_m^{n+1} = \frac{1}{\sum S_i} \sum S_i \hat{\mathbf{u}}_i^{n+1} \quad (31)$$

The Lagrangian nodes are then translated with the mean interfacial velocity:

$$\hat{\mathbf{x}}_i^{n+1} = \hat{\mathbf{x}}_i^n + \Delta t \hat{\mathbf{u}}_m^{n+1} \quad (32)$$

The phase indicator is integrated using the new front position by a geometrical procedure $\mathcal{G}()$:

$$I^{n+1} = \mathcal{G}(\hat{\mathbf{x}}^{n+1}) \quad (33)$$

And finally the physical properties are updated:

$$\rho^{n+1} = I^{n+1} \rho_{solid} + (1 - I^{n+1}) \rho_{fluid} \quad (34)$$

$$\mu^{n+1} = \begin{cases} \mu_{solid} & \text{if } I^{n+1} = 1 \\ \mu_{fluid} & \text{if } I^{n+1} < 1 \end{cases} \quad (35)$$

The algorithm is implemented in the TrioCFD code developed by CEA relying on the TRUST platform (formerly known as Trio_U). The code is fully parallel, written in C++ and has been widely used to simulate both single-phase and multi-phases (liquid/gas) flows (Toutant and Bataille (2013); Aulery et al. (2015); Dupuy et al. (2018, 2019); du Cluzeau et al. (2019, 2020, 2022)).

3. Canonical validation cases

In this section, the validity of the present method is demonstrated by comparing its performances to reproduce the experimental data of ten Cate et al. (2002) and Gondret et al. (2002).

Case	ρ_s/ρ_f	ρ_f [kg.m ⁻³]	μ_f [Pa.s]	V_{inf} [m.s ⁻¹]	Re
1.1	1.115	970	0.373	0.038	1.5
1.2	1.161	965	0.212	0.060	4.1
1.3	1.164	963	0.113	0.091	11.6
1.4	1.167	960	0.058	0.128	31.9

Table 1: Physical parameters for a spherical particle settling in viscous fluid

3.1. Free-falling sphere

The first validation case considered to be the settling of spherical a particle in a three-dimensional box at different Reynolds numbers. The test case is based on the experimental configuration of ten Cate et al. (2002) where a single sphere, of diameter $dp = 15 \text{ mm}$, is released at rest in an open quiescent container. This numerical benchmark was also done by Vincent et al. (2014); Zhou et al. (2017); Chen and Müller (2020). Reynolds numbers, $Re_t = \rho_f V_t R_p / \mu_f$ with V_t the terminal velocity, of 1.5, 4.1, 11.6 and 32.2 are considered by adjusting the fluid viscosity inside the box as shown in Tab. 1. The container dimensions are $0.1 \times 0.16 \times 0.1 \text{ m}^3$ in the x, y and z-direction respectively. The gravity $g = 9.81 \text{ m.s}^{-1}$ acts in the negative y-direction. The release position of the particle gravity center is positioned 12.75 cm above the bottom of the tank, and centered on the x and z directions. The density of the solid particle is $\rho_p = 1120 \text{ kg.m}^{-3}$. Our numerical domain corresponds to the experimental container size. No-slip boundary conditions are imposed on the walls of the do-

main, while outflow boundary conditions (with a null reference pressure) is applied on the upper boundary. Initially, the fluid is at rest in the domain. The latter is divided into $100 \times 160 \times 100$ mesh cells, which leads to a mesh resolution of $Nd = 15$ grid cells per diameter. The viscosity ratio is set to $R_\mu = 1000$ for all the four cases. Finally, an integration time step equal to $\Delta t = 10^{-4}$ s is used for the pressure solver. Fig. 5 compares the evolution of the simulated particle vertical velocity and position to the experimental results. The velocity history of the particle highlights four different phases: (i) An acceleration phase – where the speed of the particle increases gradually until it reaches its terminal velocity –, (ii) A stationary phase – during which the particle velocity remains constant –, (iii) A deceleration phase – as the particle gets closer to the bottom wall, its velocity decrease under the effect of the viscous constraints –, (iv) A contact phase when the motion of the particle ends. With our method, the acceleration and deceleration phases are qualitatively well captured. However the method seems to underestimate the drag constraints, as the computed terminal velocity in the equilibrium phase is systematically slightly higher than the reference. As a result, the collision with the bottom of the tank occurs earlier in our simulations. Moreover, at low Reynolds number, when the particle comes into contact with the wall, an abrupt change in the slope of the velocity is noticed.

Finally, by reproducing these cases, we demonstrate that our method is able to reproduce the settling of a solid sphere in a quiescent flow. This case allows, moreover, to validate the implementation of the rigid body motion in the particle and the collision model for the no-bouncing contact regime.

3.2. Bouncing motion of a solid sphere colliding onto a planar surface in a viscous fluid

the second validation case is dedicated to the bouncing collision regime. To this end, we reproduce the experimental data of [Gondret et al. \(2002\)](#) exploring the bouncing motion of a solid sphere colliding onto a planar surface in a viscous fluid as conducted. The same benchmark was also performed by [Jain et al. \(2019\)](#); [Kidanemariam and Uhlmann \(2014\)](#); [Elghannay and Tafti \(2016\)](#). A stainless steel particle is released in a tank filled with silicon oil RV10. Under the effect of gravity, the particle accelerates towards the bottom of the tank until multiple collisions are observed. The simulated time evolution of the trajectory and vertical velocity profiles are compared to the experimental data. The simulation is conducted in a $9 \times 12 \times 9$ mm³ domain with a mesh resolution $d_p/\Delta x = 20$. The particle is 3 mm

in diameter, and its center is positioned at the coordinates (4.5 mm, 8.88 mm, 4.5 mm). The densities of the fluid and the solid are equal to 935 and 7800 kg/m³ respectively. The fluid viscosity is equal to 0.01 Pa.s and the viscosity ratio R_μ is kept to 1000. No-slip boundary conditions are imposed on all the walls of the domain. The time step is equal to 5×10^{-5} s. The advection time, defined with the terminal velocity and the mesh size, is equal to 5×10^{-3} s. To decrease the numerical costs, the simulation begins at the second rebound of the [Gondret et al. \(2002\)](#) experiments. This approach is justified because the impact of the fluid perturbation induced by the first rebound does not carry over to the following rebounds, as stated in [Gondret et al. \(2002\)](#).

Fig. 6 shows the time evolution of the particle gravity center and its settling velocity. The simulated trajectory agrees convincingly with the experimental data during the initial settling phase. The trajectory after the first rebound is properly reproduced. However slight discrepancies are observed with the experimental data for the following rebounds. This is to be expected, as experimental data are more scattered at lower Stokes numbers (see Fig. 2). As the restitution coefficient underestimation accumulates over the successive rebounds, numerically the particle comes at rest slightly sooner than in the experiments. The Stokes numbers of the successive rebounds are respectively $St = 76.1$, $St = 41.2$, $St = 18.9$ and $St = 5.2$.

Finally, this case allows extending our validation of the collision model to the bouncing regime. As the particle-wall and particle-particle collisions are treated the same way in our model (see Sec. 2), we consider at this point our model validated and in the next section we assess its capability to model complex flows involving a large number of particles.

4. Particle resolved direct numerical simulation of a 2100 liquid–solid fluidized bed

In this section, our aim is to examine the overall accuracy of the framework to reproduce the global behavior of a dense fluid-particles suspension. To do so, we report simulation results of a 2100 particles fluidized bed at 4 different fluidization velocities. The parameters for the simulation are derived from the experiment of [Aguilar-Corona \(2008\)](#) who investigated the fluidization of 6 mm monodisperse spherical particles of Pyrex ($\rho_p = 2230$ kg/m³) in a concentrated aqueous solution (65 % w/w) of potassium thiocyanate ($\rho_f = 1400$ kg/m³, $\mu_f = 3.8 \times 10^{-3}$ Pa.s). The experimental setup was designed to facilitate the validation of numerical method. The refractive index matching of

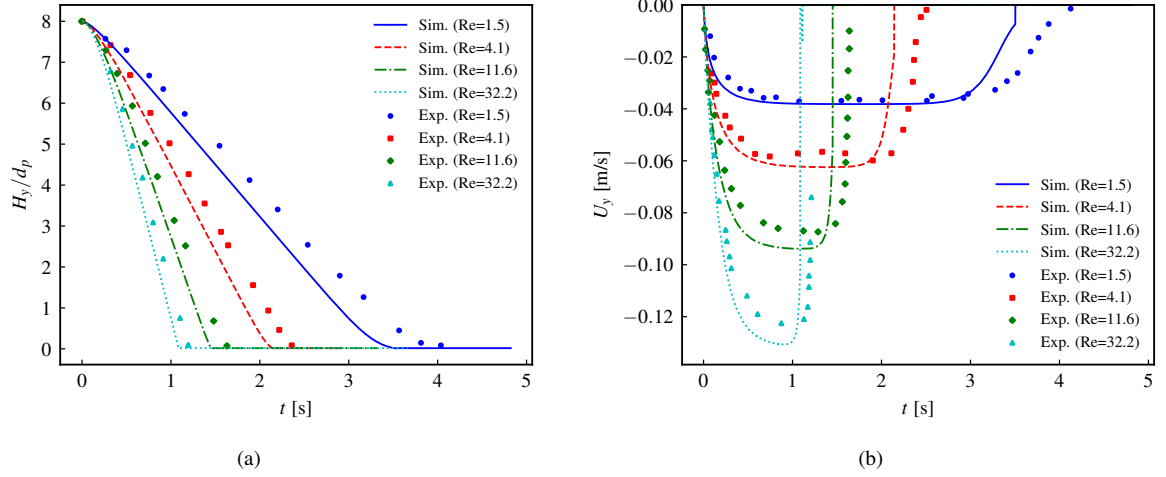


Figure 5: Time histories of the vertical position and velocity for a particle settling in a small container: (a) Normalized gap height H_y/d_p ; (b) Settling Velocity U_y . Symbols: experimental data [ten Cate et al. \(2002\)](#), lines: present simulations

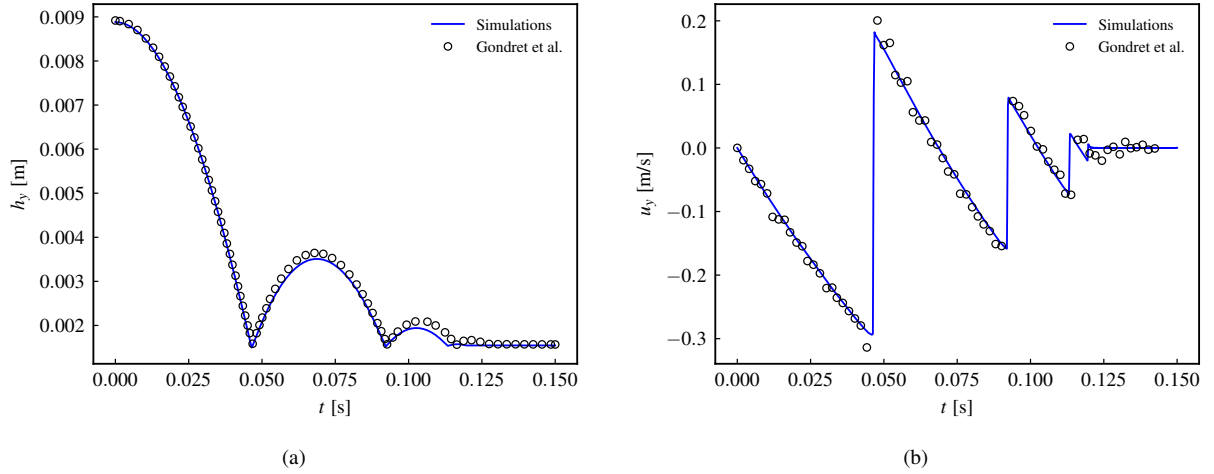


Figure 6: Time histories of the vertical position and velocity for a 3 mm steel sphere colliding with a normal surface in silicon oil RV10: (a) Vertical position h_y ; (b) Settling Velocity u_y . Symbols: experimental data [Gondret et al. \(2002\)](#), lines: present simulations

both phases allows the authors to use non-intrusive optical measurement technique (PIV) to characterize the fluid velocity field and the particles agitation. The particle terminal velocity is $V_t = 0.24 \text{ m.s}^{-1}$ (see [Aguilar-Corona \(2008\)](#)) and the associated Reynolds and Stokes numbers are 530 and 94, respectively. Note that [Ozel et al. \(2017\)](#) use a different definition of the Stokes number $St = \frac{8\rho_p}{3\rho_f Cd}$. With this definition, the Stokes number is equal to 5.3. The two definitions are equivalent if

$Re \ll 1$ and consequently $Cd = 24/Re$. Both phases are contained in a cylindrical shaped tank.

This configuration was already studied numerically by [Ozel et al. \(2017\)](#) – using the Implicit Tensorial Penalty Method of [Vincent et al. \(2014\)](#) – with a mesh resolution of $Nd = 12$. To assess the performance of our approach, we reproduce in this section the numerical configuration of Ozel for four different fluidization velocities: 0.15 m.s^{-1} , 0.12 m.s^{-1} , 0.09 m.s^{-1} and

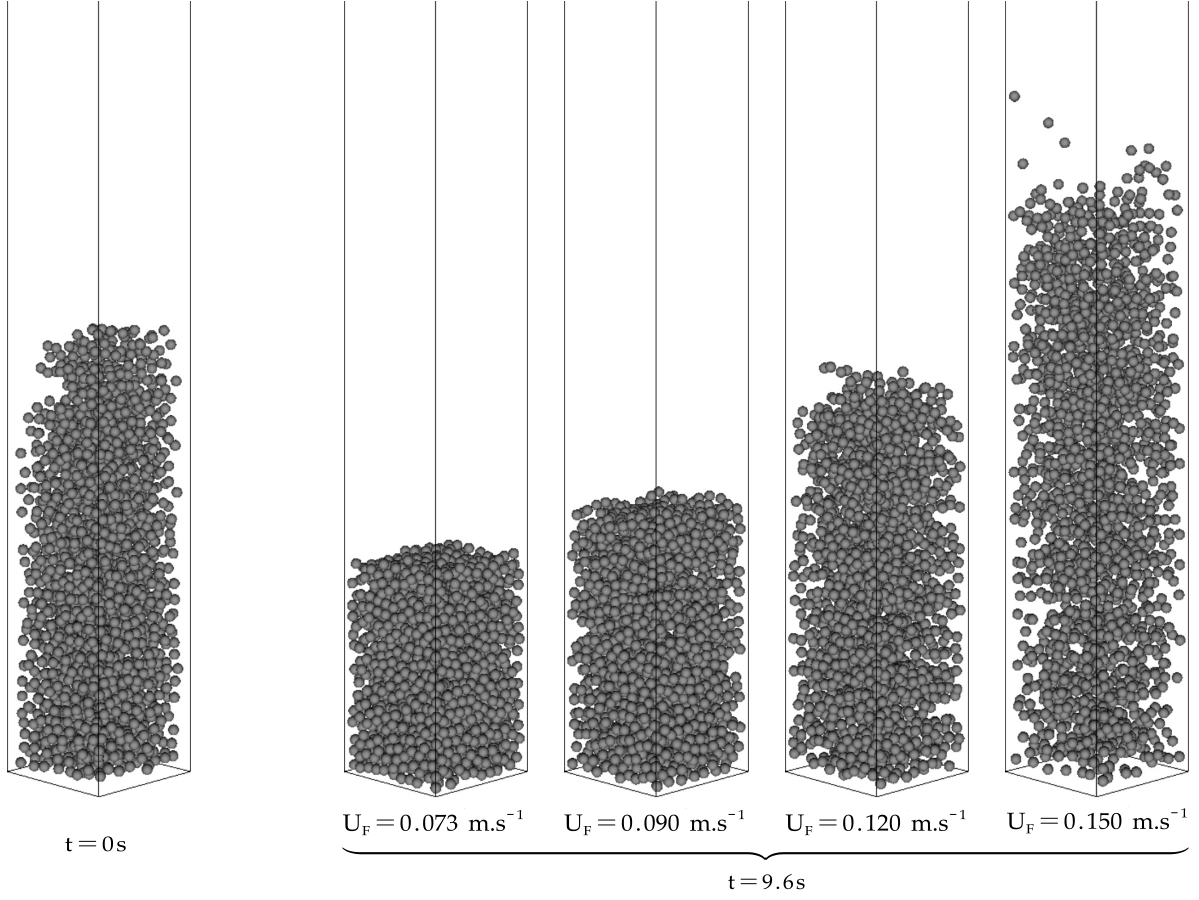


Figure 7: 3D views of the particles' position distribution in the domain for $t = 0$ s and $t = 9.6$ s for the four fluidization velocities tested.

0.073 m.s^{-1} . However, as our code does not handle O-grid mesh, the container geometry considered is a cuboid of dimensions $0.072 \times 0.648 \times 0.072$ (matching the experimental cross-section area). The simulations were performed on the same mesh resolution as Ozel, imposing $Nd = 12$. This is slightly coarser than the resolution used for the previous cases, but it appears to be a fair balance between computational cost and accuracy for this numerical case. The viscosity ratio is set to $R_\mu = 10000$. To speed up the initial transient in the simulations, particles are initially positioned so that the initial bed height approximately matches the one expected at stationary state (based on the results of Ozel et al. (2017) for a fluidization velocity of $U_F = 0.12 \text{ m.s}^{-1}$). Fig. 7 shows the initial position of the particles (left) and a snapshot at $t = 9.6$ s for the four fluidization velocities (right).

The time-evolution of the maximum particles position $y_{max}(t)$ at various fluidization velocities is shown in

Fig. 8 along side of a box plot for the fluctuation of y_{max} . This quantity is calculated by tracking the maximum y-coordinate of the center of gravity for all particles. Since the expected height of the bed at $U_F = 0.12 \text{ m.s}^{-1}$ was used to initialize the position of the particles, the transient in this case is the shortest. We can see that y_{max} fluctuates around a mean value, and that the fluctuations amplitudes increase with the fluidization velocities. The height evolution shows that a statistical stationary state is reached, roughly after 2 s, for $U_F = 0.09 \text{ m.s}^{-1}$ and $U_F = 0.073 \text{ m.s}^{-1}$. However, even after 10 s of simulation, the bed-level oscillations are quite strong for $U_F = 0.15 \text{ m.s}^{-1}$. In this case, single particles are ejected much higher than the average bed height (see Fig. 7).

Fig. 9 shows the time averaged evolution of the solid fraction α as a function of the height y , alongside a box plot showing the spread of the values of the volume fraction relative to the mean. These profiles were obtained

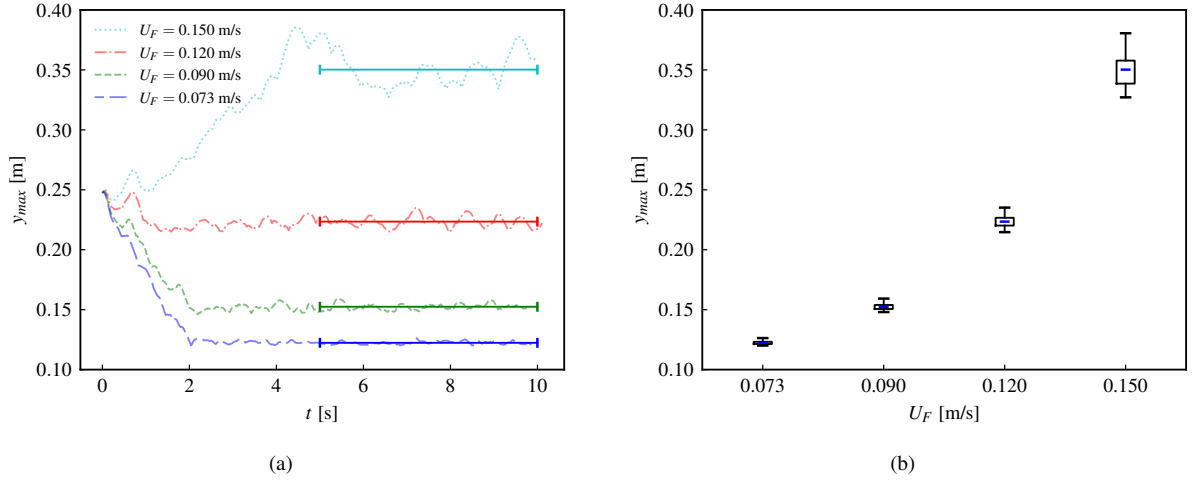


Figure 8: (a): Time-evolution of maximum axial particle position at different fluidization velocities: $U_F = 0.15, 0.12, 0.09, 0.073 \text{ m.s}^{-1}$. The continuous lines represent the average mean value of y_{max} over the range $t = [5 \text{ s}, 10 \text{ s}]$ (b) Box plot of the distribution of y_{max} (m). The box represents the interquartile range (IQR), the line inside the box is the mean, the whiskers extend to the minimum and maximum values.

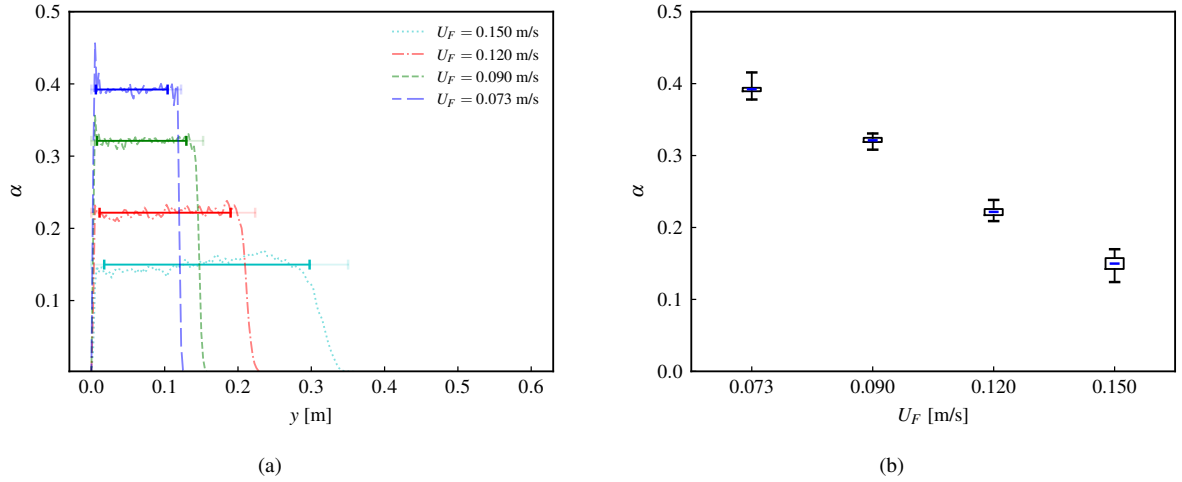


Figure 9: (a) Time-section average of solid void fraction α as a function of height. The continuous lines represent the mean value of α over $y = [0.05\overline{y_{max}}, 0.95\overline{y_{max}}]$. (b) Box plot of the distribution of α . The box represents the interquartile range (IQR), the line inside the box is the mean, the whiskers extend to the minimum and maximum values.

by taking cross sections of the domain at regular intervals and calculating the mean solid fraction over the cross section. The instantaneous profiles obtained were then time averaged over the period $[t_0 = 5 \text{ s}, t_1 = 10 \text{ s}]$ to obtain the time averaged profiles shown in Fig 9. From both figures, One can see that the volume fraction is fairly uniform along the height of the bed; how-

ever, a transition zone appears between the bed itself and the pure fluid region. We can see that the thickness of this transition zone directly depend on the fluidization speed. The lower the fluidization velocity, the narrower the transition zone. Indeed, this transition zone is nothing but a time average of the fluctuation of the bed height observed on Fig. 7 and 8. The bed volume frac-

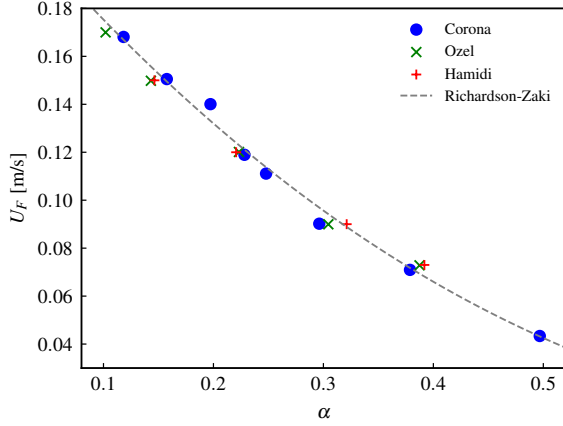


Figure 10: Fluidization velocity with respect to the bed solid concentration.

tion is calculated by taking the spatial average along the y direction between $[0.05\bar{y}_{max}; 0.95\bar{y}_{max}]$ to eliminate the edge effects caused by the wide transition zone at high fluidization speeds. $\bar{y}_{max}$ is the time averaged maximal axial particle position given by:

$$\bar{y}_{max} = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} y_{max}(t) dt$$

The resulting average bed volume fraction is plotted against the fluidization velocity, on Fig. 10, and compared with the experimental data. of Aguilar-Corona (2008) the numerical results of Ozel et al. (2017) and the empirical correlation proposed by Richardson and Zaki (1954) (for $n = 2.4$ and $U_{F0} = 0.24 \text{ m.s}^{-1}$ as proposed by Aguilar-Corona (2008)) given by:

$$\frac{U_F}{U_{F0}} = (1 - \alpha)^n \quad (36)$$

where U_F is the fluidization velocity, U_{F0} is the entrainment velocity and n is a function of Re_t .

$$\begin{cases} n = 4.65 & \text{if } Re_t < 0.2 \\ n = 4.4Re_t^{0.03} & \text{if } 0.2 < Re_t < 1 \\ n = 4.45Re_t^{0.1} & \text{if } 1 < Re_t < 500 \\ n = 2.4 & \text{if } Re_t > 500 \end{cases} \quad (37)$$

One can observe in Fig. 10 that our results are in good agreement with both the numerical and experimental references. All the evolutions were well predicted by the empirical correlation for the given n and U_{F0} values. Fig. 11 displays a color map of the velocity magnitude, at the center plan of the domain. One can observe that the velocity in the particles is one order of magnitude

lower than the fluid velocities. As the fluidization velocities increase, larger pseudo-turbulent structures emerge behind the particles. The interaction of the developing wakes with the particles results in a complex flow dynamic. A more quantitative insight of this flow configuration is detailed in the following.

4.1. Solid phase agitation

A much challenging validation relies on the ability of the method to predict the velocity statistics of the solid phase and especially its agitation. Statistical quantities are computed using the same methodology as in the reference data. The instantaneous variance of particle velocity in each direction i are first calculated using Eq. 38:

$$\langle \tilde{u}_{p,i}^2 \rangle_p = \left\langle \left(u_{p,i} - \langle u_{p,i} \rangle_p \right)^2 \right\rangle_p \quad (38)$$

The notation $\langle \cdot \rangle_p$ denotes the particle phase average :

$$\langle \phi_p \rangle_p = \frac{1}{N_p} \sum_{i=1}^{N_p} \phi_p \quad (39)$$

where N_p is the total number of particles in the domain. Then, the time average of the variance of the particle velocities (Eq. 40) is computed for all directions and shown in Fig. 12 alongside the previous experimental and numerical results.

$$\langle \tilde{u}_{p,i}^2 \rangle = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \langle \tilde{u}_{p,i}^2 \rangle_p dt \quad (40)$$

We can see that our method allows to accurately predict the velocity variance, for the three components, for solid fractions $\alpha > 0.2$. The superimposition of the two transverse components, x and z , attest the convergence of the statistics. For the lowest volume fraction (highest fluidization speed), our simulation overestimates the variance of the three components and the two transverse components are no longer matching. Moreover, the variance of the velocity along the vertical axis is always higher than in the transverse direction whatever the solid fraction. This anisotropy can be characterized by a coefficient k_{anis} :

$$k_{anis} = \sqrt{\frac{\langle \tilde{u}_{p,y}^2 \rangle}{\frac{1}{2} (\langle \tilde{u}_{p,x}^2 \rangle + \langle \tilde{u}_{p,z}^2 \rangle)}} \quad (41)$$

The evolution of the anisotropy coefficient as a function of the volume fraction is plotted in Fig. 13. We can see that, even if the values obtained are slightly lower than Ozel et al. (2017), as expected we find

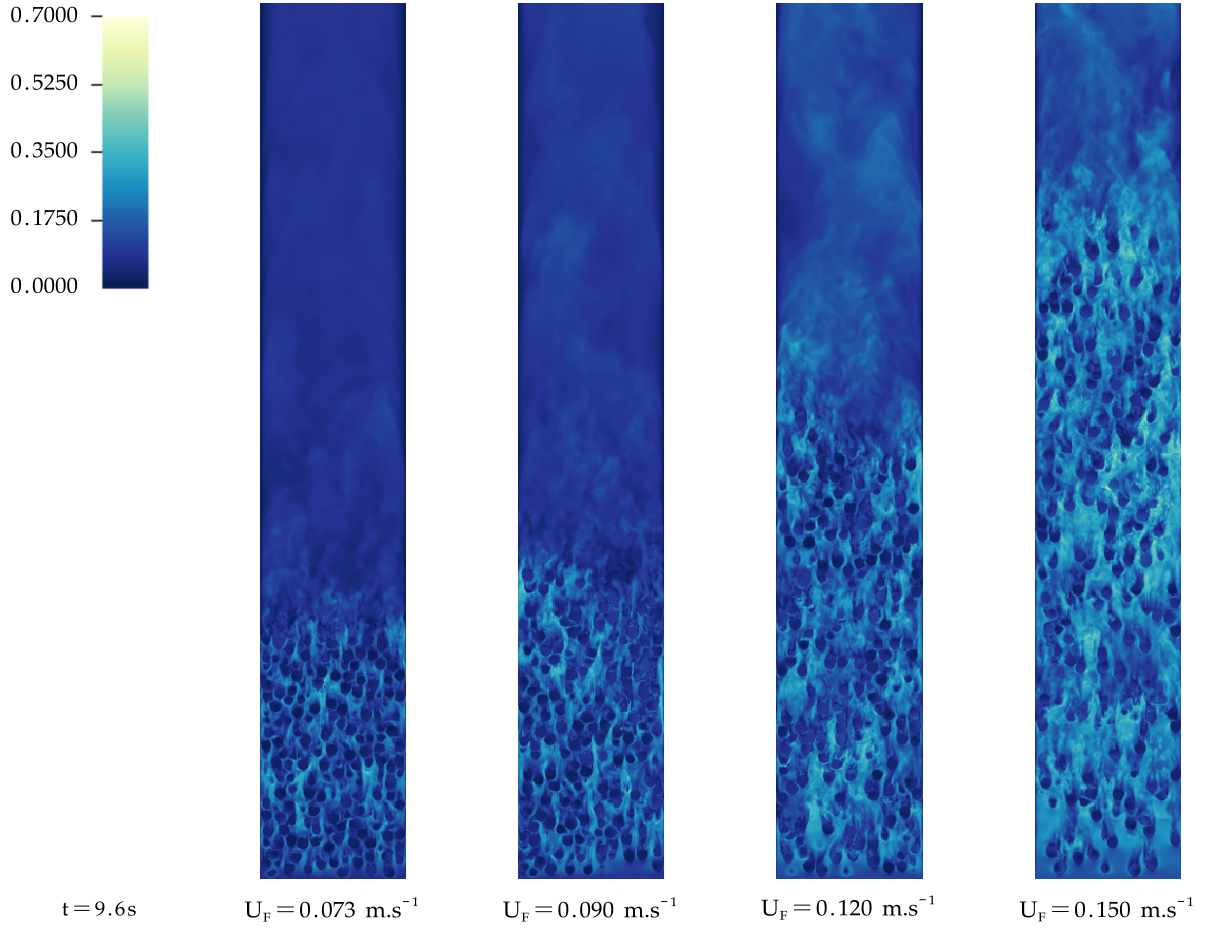


Figure 11: Contours of the velocity magnitude, in a plane centered in the domain of the x-direction, in the established phase ($t = 9.6\text{ s}$) and for the four fluidization velocities U_F .

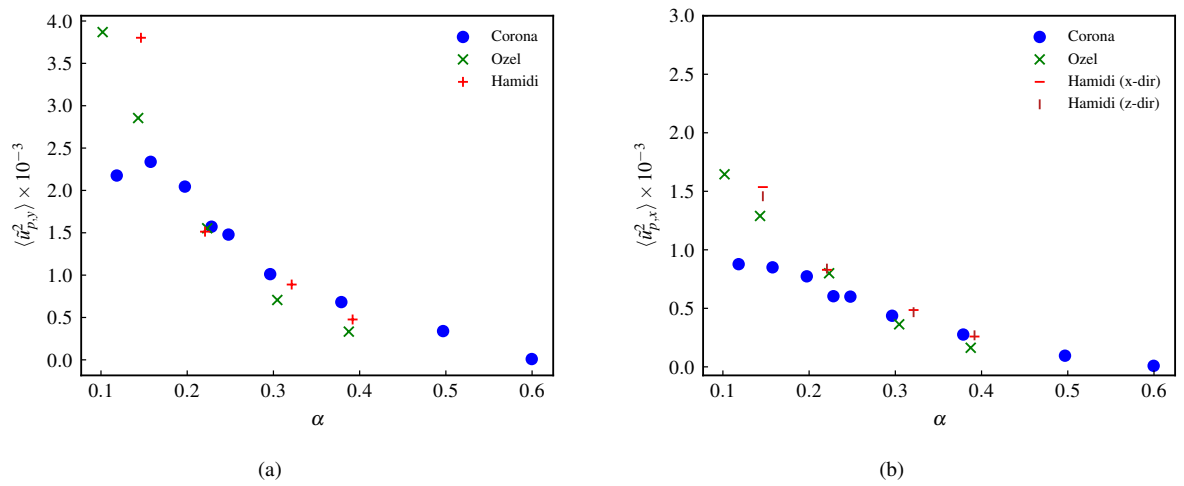


Figure 12: Variance of axial (a) and transverse (b) particle velocity with respect to the bed solid concentration.

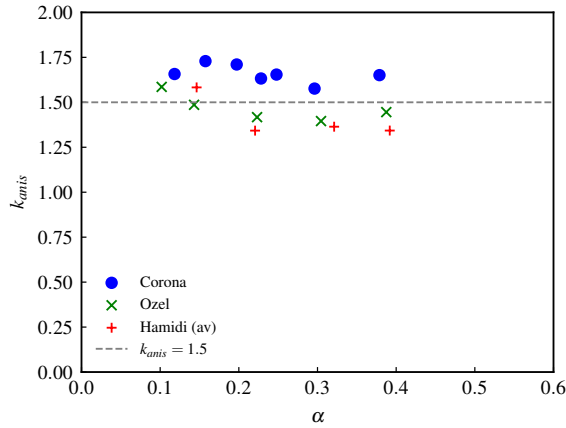


Figure 13: Anisotropy coefficient of the particle velocity fluctuations as a function of the bed solid concentration

no dependence of the k_{anis} on the averaged particle volume fraction (overlooking the non-converged case which corresponds to the highest fluidization velocity $U_F = 0.15 m.s^{-1}$). Based on this analysis, the accuracy of our approach is comparable to that of [Ozel et al. \(2017\)](#); [Vincent et al. \(2014\)](#).

5. Conclusion

We have implemented in the Front-Tracking framework a one-fluid method capable of performing Particle-resolved direct numerical simulations of dense fluid-particle flow. The interactions between the fluid and the particles are taken into account by a combined viscous penalty method and a front tracking algorithm. Both collision and lubrication interactions are simultaneously modeled by soft sphere collision model similar to what [Mohaghegh and Udaykumar \(2019\)](#) proposed. During a collision, the spring stiffness of the model is adjusted to obtain the desired rebound velocity by using experimental correlation relating the impact Stokes number to the coefficient of restitution. This approach allows to avoid using additional closure laws for lubrication modeling, which results in a reduction of the number of numerical parameters in the models. The method has been tested against well-established experimental benchmarks of, and demonstrated good overall numerical consistency. The hydrodynamics was first validated by simulating the motion of a settling sphere in a fluid. The method showed qualitatively good results with the experiments on the range of terminal Reynolds numbers studied ($1.5 < Re < 32$). The collision modeling was

then validated by reproducing the bouncing trajectory of a spherical particle colliding into a planar surface. The method proved to be quite capable of reproducing a physically realistic bouncing motion. Finally, the ability of the method to simulate granular flow with numerous particles (> 2000) was demonstrated by reproducing the experiments and [Aguilar-Corona \(2008\)](#). The results obtained showed quantitative consistency with the references for solid fraction ranging from 0.2 to 0.4. In this range, our method showed similar performances to the one developed by [Ozel et al. \(2017\)](#). Overall the proposed numerical approach does capture convincingly the physics of particles–fluid and inter-particle interactions and was shown to be valid over a wide range of Stokes/Reynolds numbers.

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