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A second-order accurate Immersed Boundary Method combined with a soft-sphere collision model for fully-resolved simulations of particle-laden flows

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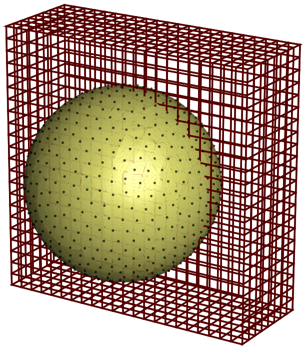
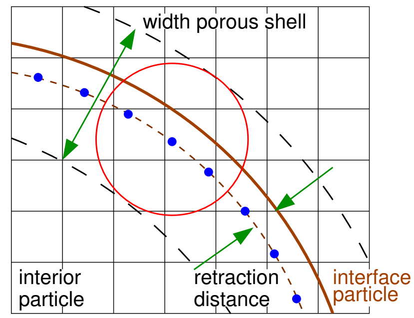
ABSTRACT

1. Introduction. Flows laden with solid particles are abundant in nature and industry. Examples are the transport of dense sand-water mixtures through pipes for land reclamation purposes, natural erosion and sediment transport in rivers, fluidized bed reactors for the gasification of biomass or coal and the flocculation/sedimentation process in the treatment of drinking water. In all these examples the flow is turbulent, the particles may have a finite size (*i.e.*, a size larger than the Kolmogorov scale of the turbulent flow) and the solid volume fraction may be large ($> 10^{-3}$) such that particle collisions are significant. The structure and dynamics of such flows are rather complex. Though the governing equations for the fluid flow and particle motions are known for a long time, yet little is understood of their physics. For instance, no reliable model exists that can accurately predict the friction factor for dense sediment transport through pipes. Thanks to the development of efficient computational methods and the ever increasing computing power, Direct Numerical Simulation (DNS) of particle-laden flows has recently become in reach and will open a new window on their physics. The goal of our research is to use DNS to improve our understanding of dense particle-laden turbulent flows through plane channels and circular pipes.
The Immersed Boundary Method (IBM) [1, 2] has become a popular method for DNS of particle-laden flows. Characteristic for IBM is that the computational grid for the fluid phase does not conform to the shape of the particles like in conventional methods with a body-fitted grid. The computational grid is fixed in time, continuous in space and often Cartesian. Instead of imposing explicit no-slip/no-penetration (ns/np) conditions at the fluid/particle interface, forces are added to the flow field near the interface such that the ns/np conditions are satisfied by good approximation. The advantage of the IBM over a method with a body-fitted grid is its computational efficiency: it does not require regridding when particles are moving and a Cartesian grid enables the use of efficient discretization schemes and flow solvers. The challenge is to develop IBM that are not only efficient, but also accurate.
Our DNS is based on a second-order accurate IBM [3] combined with a soft-sphere collision model [4] for accommodating particle collisions and lubrication force corrections for particles at very close distance [5]. The overall model is currently tested for oblique collisions of a sphere onto a plane wall. At the colloquium we will give an overview of the IBM and the collision model with lubrication force corrections. Below a brief summary is given.

2. Original IBM. Our IBM is based on the direct-forcing IBM of Uhlmann [6] and is embedded in a finite-volume/pressure-correction method. The IBM makes use of two different grids: a 3D Cartesian grid for the fluid phase and a quasi-2D uniform grid attached to and moving with the surface of the particles as illustrated in Fig. 1.a. The grids are referred to as the Eulerian and the Lagrangian grid, respectively. The method solves the Navier-Stokes equations for the fluid phase and the Newton-Euler equations for the particles. The flow-induced force and torque acting on a particle is obtained from the IBM force distribution on the Lagrangian grid. The IBM force distribution on the Lagrangian grid is computed from the requirement that on the surface of the particle the provisional fluid velocity in the pressure-correction scheme is equal to the local particle velocity. Since the grid points of the two grids do not overlap, interpolation is required of the provisional velocity from the Eulerian to the Lagrangian grid. Furthermore, spreading is required of the computed IBM force from the Lagrangian back to the Eulerian grid. In Uhlmann's IBM the interpolation and spreading operations are based on the regularized Dirac delta function of Roma et al. [7] with a width of three Eulerian grid cells. Consequently, the particles have a smooth (non-sharp) interface from the point of view of the fluid phase. In fact, they are covered by a *porous shell* as illustrated in Fig. 1.b.
The regularization of the Dirac delta function has the important advantage of suppressing undesired high-frequency oscillations in the force and torque acting on a particle when it moves over the Eulerian grid. These oscillations originate from variations in the interpolated provisional velocity when the Lagrangian grid moves with the particle over the Eulerian grid and thus changes its orientation relative to the Eulerian grid. In other words, they are present because the interpolation operation is not translation invariant [1]. We refer to this phenomenon as *grid locking*, since the wavelength of the oscillations is set by the dimensions of the Eulerian grid cells and their period by the time it takes for a particle to travel from one Eulerian grid cell to another. Uhlmann [6] showed for the case of a forced oscillation of a cylinder in uniform cross-flow that the amplitude of the spurious oscillations decreases when the width of the regularized Dirac delta function is increased. The regularized Dirac delta function of Roma et al. [7] with a width of three Eulerian grid cells is considered as effective for suppressing grid locking and its compact support as computationally efficient [6].
However, the regularization of the Dirac delta function has also a major disadvantage. The interpolation of the provisional velocity based on the regularized Dirac delta function approach is formally second-order accurate in space, but only when applied to a smooth velocity field. Peskin [1] pointed out that the velocity field near a solid boundary is non-smooth as it contains a jump in its normal derivative over the boundary. Consequently, the interpolation of the provisional velocity becomes fist-order accurate. A possible way to improve the accuracy is to resort to a sharp representation of the interface. However, this will probably amplify grid locking, which is undesired. The challenge is to keep a smooth representation of the interface in order to suppress grid locking and to find other ways for improving the accuracy of the IBM.



(a)



(b)

Figure 1: (a) Illustration of Eulerian and Lagrangian grid for $D/\Delta x = 16$, where D is the sphere diameter, and retraction distance $r_d = 0.3\Delta x$. (b) Illustration of porous shell around a sphere. Circle indicates the spatial extent of the regularized Dirac delta function. Dots indicate the Lagrangian grid, which is being retracted from the actual surface of the sphere (black line) by a radial distance r_d.

3. Modified IBM with second-order accuracy and suppression of grid locking. Recently, Breugem [3] demonstrated that the accuracy of the IBM can actually be increased to second order by a slight retraction of the Lagrangian grid from the surface towards the interior of a spherical particle. The smooth representation of the particle interface is retained and thus grid locking is still suppressed. The optimal retraction distance was empirically found to be close to $r_d = 0.3\Delta x$. This has been demonstrated for many different flows over a range of Reynolds numbers such as flow through a fixed array of spheres, a freely moving sphere in plane Poiseuille flow, two spheres in squeezing motion at a gap width of $D/4$ and the drafting-kissing-tumbling interaction between two spheres. The retraction of the Lagrangian grid compensates for the excess in the effective particle diameter due to the smooth representation of the interface (i.e., due to the presence of a porous shell).

Next to the retraction of the Lagrangian grid, our IBM also contains two other modifications of the original method: (1) the improvement of the approximation of the ns/np condition at the particle interface by the multidirect forcing scheme of Luo et al. [8] and (2) an enhanced numerical stability for particle-fluid mass density ratios near unity by a direct account of the inertia of the fluid contained within the particles [9].

4. Lubrication corrections. As mentioned above, the second-order accuracy of our IBM has been demonstrated among others for two spheres in squeezing motion at a normalised gap width $\varepsilon = (D/4)/R = 0.5$. However, because our IBM makes use of a fixed Cartesian grid for the fluid phase, the method will eventually fail to capture the intervening film and hence the lubrication force when the two spheres are at very close distance. For that reason lubrication force and torque corrections have been added to the Newton-Euler equations for the particle motion when two particles are within a certain threshold distance from each other. The threshold gap width (ε_{lc}) at which the lubrication correction is activated has been determined from numerical simulations.

Figure 2.a shows the normalized lubrication force for the case of two equal spheres in squeezing motion as function of the normalized gap width. The simulation results are compared with the analytical solution from Brenner [10]. For $D/\Delta x = 16$ the simulation results deviate from the analytical result for $\varepsilon \lesssim 0.25$, which corresponds to a gap width $\lesssim 2\Delta x$. When the grid resolution is increased to $D/\Delta x = 32$ the agreement with the analytical result is good down to $\varepsilon \approx 0.025$. The good agreement till $\varepsilon \approx 0.025$ is quite remarkable, since it corresponds to a gap width of $\approx 0.4\Delta x$, which is significantly smaller than the grid spacing. For smaller gap width the numerical solution is unable to capture the analytical solution, which diverges to ∞ for $\varepsilon \to 0$. Figure 2.b shows the same simulation results as depicted in Fig. 2.a, but now including a lubrication force correction. This correction is based on an asymptotic expansion of Brenner's analytical solution for small ε [5]. The agreement between the corrected simulation data and the analytical result is now good over the whole range of ε, in particular for the highest resolution. A similar lubrication force correction has been implemented in our model for a sphere moving perpendicular to a plane wall.

The asymptotic expansions of λ for two spheres in squeezing motion and for the head-on collision of a sphere onto a plane wall diverge to ∞ for $\varepsilon \to 0$. This will actually prevent any solid contact. However, the asymptotic expansions have been derived for a perfectly smooth and rigid sphere/wall and are based on the assumption that the Stokes equations still hold for the flow in the intervening film when $\varepsilon \to 0$. From experiments it is known that surface roughness elements of the sphere/wall cause actual sphere-sphere/wall contact when the gap width (εR) is on the order of the typical size of the surface roughness elements [11]. This will hamper further drainage of the intervening film and the drainage process will eventually stop when many roughness elements have made contact with each other. This effect is modelled by fixing the lubrication correction at $\lambda(\varepsilon) = \lambda(\varepsilon_1)$ for $-\varepsilon_2 \leq \varepsilon \leq \varepsilon_1$, where $\varepsilon_1 = 10^{-3}$ and $\varepsilon_2 = 10^{-2}$ are empirical constants. For $\varepsilon \leq -\varepsilon_2$ the lubrication force correction is turned off.

5. Soft-sphere collision model. The lubrication correction model has been combined with a soft-sphere collision model [4] to compute the collision force between particles once solid contact has been made ($\varepsilon \leq 0$). This is illustrated in Fig. 3 for a sphere colliding on a plane wall. In the soft-sphere collision model particles are allowed to slightly overlap with each other. The contact force is computed from the overlap between the particles and their relative velocity. The collision force is decomposed into a normal and tangential component, where the normal component is parallel to the unit normal on the particle interface at the point of contact. The model has been tested for head-on collision of a sphere onto a plane wall in a closed cavity filled with a viscous fluid. It was demonstrated that the soft-sphere collision model combined with lubrication force corrections can reproduce available experimental data for the coefficient of restitution as function of the impact Stokes number [5, 12]. Currently, we are testing the model for oblique collisions.

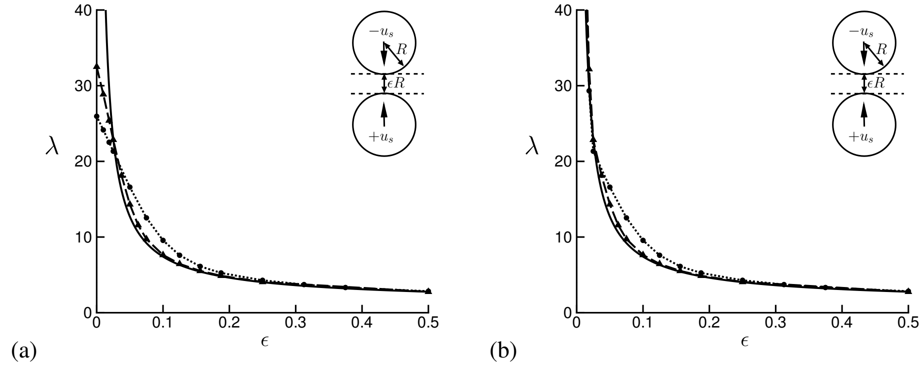


Figure 2: (a) The Stokes amplification factor $\lambda \equiv F_d/(6\pi\mu R u_s)$ as function of normalized gap width ε for two equal solid spheres in squeezing motion. Dots and dotted line: results from the IBM simulations at grid resolution $D/\Delta x = 16$. Triangles and dashed line: results from the IBM simulation at $D/\Delta x = 32$. Solid line: analytical solution from Brenner [10]. (b) Idem as in (a), but now with the lubrication force correction for $\varepsilon \leq \varepsilon_{lc}$.

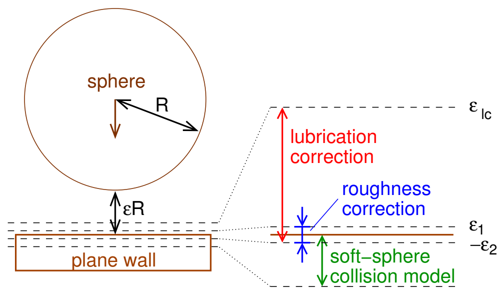


Figure 3: Illustration of the soft-sphere collision model combined with a lubrication correction for the head-on collision of a sphere onto a plane wall. The parameters ε_{lc}, ε_1 and ε_2 are explained in the text.

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