Revisiting the use of the immersed-boundary lattice-Boltzmann method for simulations of suspended particles

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The immersed-boundary lattice-Boltzmann method (IB-LBM) is increasingly being used in simulations of dense suspensions. These systems are computationally very expensive and can strongly benefit from lower resolutions that still maintain the desired accuracy for the quantities of interest. IB-LBM has a number of free parameters that have to be defined, often without exact knowledge of the tradeoffs, since their behavior in low resolutions is not well understood. Such parameters are the lattice constant Δx, the number of vertices Nv, the interpolation kernel φ, and the LBM relaxation time τ. We investigate the effect of these IB-LBM parameters on a number of straightforward but challenging benchmarks. The systems considered are (a) the flow of a single sphere in shear flow, (b) the collision of two spheres in shear flow, and (c) the lubrication interaction of two spheres. All benchmarks are performed in three dimensions. The first two systems are used for determining two effective radii: the hydrodynamic radius rhyd and the particle interaction radius rinter. The last system is used to establish the numerical robustness of the lubrication forces, used to probe the hydrodynamic interactions in the limit of small gaps. Our results show that lower spatial resolutions result in larger hydrodynamic and interaction radii, while surface densities should be chosen above two vertices per LU2 to prevent fluid penetration in underresolved meshes. Underresolved meshes also failed to produce the migration of particles toward the center of the domain due to lift forces in Couette flow, mostly noticeable for IBM-kernel φ2. Kernel φ2a, despite being more robust toward mesh resolution, produces a notable membrane thickness, leading to the breakdown of the lubrication forces in larger gaps, and its use in dense suspensions where the mean particle distances are small can result in undesired behavior. rhyd is measured to be different from rinter, suggesting that there is no consistent measure to recalibrate the radius of the suspended particle.

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I. INTRODUCTION

The immersed-boundary method (IBM) is a pure fluid-structure interaction method that has been used in a wide range of applications [1–8]. Many variations of the IBM have been presented since its original introduction by Peskin in 1972 [9,10]. Uhlmann [11] suggested an improved version of the IBM with a direct formulation of the fluid-solid interaction force, using the regularized δ function to associate arbitrary Lagrangian with discrete Eulerian positions. Kempe and Fröhlich [12] proposed several enhancements to Uhlmann’s approach [11] to improve the range of stability of the method and to deal with approaching interfaces. Yang et al. [13] developed a smoothing technique for the discrete δ functions of the IBM to suppress the nonphysical oscillations in the volume forces, while Wu and Shu [14] presented a model that accurately satisfies the nonslip boundary condition at boundary points.

However, the initial formulation of the IBM is also widely used due to its simplicity [5,15,16]. The role of some key IBM parameters and their effect on the interactions between the fluid and the immersed structure, or between the immersed structures, is not fully understood in either the initial formulation or the improved versions. Krieger et al. [17] investigated the impact of some of these relevant parameters by looking into the deformation of an initially spherical capsule, freely suspended in a simple shear flow. They found that the tessellation method and resolution of the membrane mesh play only a minor role, while the width of the discrete δ function significantly affected the results of their simulations.

The IBM is often combined with the lattice-Boltzmann method (LBM) as the fluid solver, a combination known as the immersed-boundary lattice-Boltzmann method (IB-LBM). The IB-LBM is widely used for the simulation of deformable particles, such as red blood cells (RBCs) [4–8,15,16] and capsules [17,18]. Due to their deformability, RBCs can pack very efficiently, resulting in blood suspensions with very high volume fraction in which the mean particle-particle distance is small.

To understand the role of IB-LBM parameters in particle-particle interactions, we performed an extensive study of their impact on a set of demanding benchmarks. The parameters considered are the interpolation kernel φn, the grid resolution Δx, the number of vertices used to represent a suspended particle, Nv, and the LBM relaxation parameter τ. The basic IBM implementation is used with stiff spherical particles, and any deviation from the spherical shape is being tracked. Many analytical solutions and reference tests exist or can be constructed for solid spheres [19–24], rendering them the most tractable shape for our simulations. We use the same version of the IB-LBM as the ones used in our deformable particle simulations [5,6,15] to study the behavior and shortcomings of the approach, yet in the stiff limit to approximate solid spheres. We are not using a variant for solid objects, since our aim is to study the behavior of the IBM, and spheres provide a clean method to do so. The benchmark systems are (a) a single sphere...
in shear flow, determining its effective hydrodynamic volume by measuring Einstein’s viscosity, (b) the collision of two particles in shear flow, and (c) the lubrication interaction of two spheres. All benchmarks are performed in three dimensions.

In the appendices, we provide supporting material for the results presented in the paper.

II. METHODS

A combined immersed-boundary lattice-Boltzmann method is employed to couple the suspended spheres with the fluid. The constitutive model used in the following simulations is the same as for red blood cells (RBCs) [15], yet much stiffer. Spheres are chosen for the simulations due to the existence of benchmark tests and known analytical results. The departure from the spherical shape is being tracked and ensured to be within acceptable limits (less than 1% of the radius). More information can be found in Appendix B.

A. Lattice-Boltzmann method

The lattice-Boltzmann method (LBM) is a well-established mesoscopic approach that solves asymptotically the incompressible Navier-Stokes equation [25]. The LBM’s main quantity is the set of populations \( f_i(x,t) \), which corresponds to the discretized probability distribution of finding particles in site \( x \) at time \( t \), moving with velocity \( c_i \).

The time evolution of the distributions, when an external force is involved, is given by the forced single-relaxation time LBGK equation [25, 26],

\[
f_i(x + c_i \Delta t, t + \Delta t) = f_i(x,t) - \frac{f_i(x,t) - f_i^{eq}(x,t)}{\tau} + \Delta t \mathbf{F}_i, \tag{1}
\]

where \( \tau \) is the relaxation parameter, \( \Delta t \) is the time step, \( f_i^{eq}(x,t) \) is the equilibrium population, and \( \mathbf{F}_i \) is the forcing term.

The equilibrium populations are given by

\[
f_i^{eq}(x,t) = w_i \rho \left[ 1 + c_i \cdot \mathbf{u} + \frac{1}{2} \left( \frac{\mathbf{u} \cdot \mathbf{c}_i}{c_i^2} \right)^2 - \frac{\tau}{2c_i^2} \right], \tag{2}
\]

where \( w_i \) is the weighting factor, \( \rho \) and \( \mathbf{u} \) are the fluid density and velocity, respectively, and \( c_i = \frac{1}{\sqrt{3}} \Delta x/\Delta t \) is the lattice speed of sound.

The zeroth and first moments of the populations recover the fluid density \( \rho = \sum_i f_i \) and velocity \( \mathbf{u} = \sum_i f_i \mathbf{c}_i + \frac{\mathbf{F}}{\rho} \), while the kinematic viscosity \( \nu \) of the fluid is given by \( \nu = \frac{1}{\tau} c_i^2 \Delta t \). The forcing term \( \mathbf{F}_i \) of Eq. (1) is in the form of

\[
\mathbf{F}_i = \left( 1 - \frac{1}{2\tau} \right) w_i \left( \mathbf{c}_i - \mathbf{u} \right) \cdot \left( \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_i^2} \right) \mathbf{c}_i + \left( \mathbf{c}_i \cdot \mathbf{u} \right) \cdot \left( \mathbf{c}_i - \mathbf{u} \right) \cdot \mathbf{f}, \tag{3}
\]

where \( \mathbf{f} \) is the external body force density.

We used the so-called D3Q19 model (three-dimensional with 19 velocity components) as implemented in the open-source LBM-solver Palabos [15, 27] and built the IBM and the constitutive model on top of it.

B. Constitutive model of a cell membrane

We employ the spectrin-link model [28, 29], widely used in red blood cell simulations and carefully parametrized in this study to correspond to a near-rigid sphere. Each sphere consists of a network of vertices, forming a triangular mesh. The Helmholtz free energy of the system is given by

\[
F(x_n) = F_{in-plane} + F_{bending} + F_{volume} + F_{area}, \tag{4}
\]

where \( x_n \), \( n \in 1, \ldots, N \), are the vertices of a two-dimensional triangulated network describing the surface of a sphere.

The in-plane free-energy term is written as

\[
F_{in-plane} = k_{WLC} \left( \sum_{l \in \text{edges}} V_{WLC}(L_l) + \sum_{l \in \text{edges}} \frac{k_{\text{rep}}}{L_l} \right), \tag{5}
\]

with \( V_{WLC}(L_l) = \frac{k_B T L_{\text{max}}}{4 \rho} \left( 3x_l^2 - 2x_l^4 \right) \). \tag{6}

\( V_{WLC} \) is the wormlike chain potential, \( L_l \) is the length of the edge \( l \), \( L_{\text{max}} \) is the maximum allowed extension length, \( x_l \) is defined as \( x_l = \frac{L_l}{L_{\text{max}}} \), \( p \) is the persistence length, and \( k_{\text{rep}} \) is a constant chosen so that the corresponding in-plane force is zero for the equilibrium length \( L_0 \). \( k_B \) is Boltzmann’s constant, and \( T = 300 \) K is the temperature.

The bending energy is defined as

\[
F_{bending} = \sum_{\text{adjacent } \alpha, \beta} k_{\text{bend}} \left( 1 - \cos(\theta_{\alpha \beta} - \theta_0) \right), \tag{7}
\]

where \( k_{\text{bend}} \) is the bending constant, and \( \theta_{\alpha \beta} \) and \( \theta_0 \) are the instantaneous and equilibrium angles between two adjacent triangles, respectively.

The volume and surface conservation constraints are written as

\[
F_{volume} = k_{\text{volume}} \left( \frac{k_B T}{2L_0^3} \frac{(\Omega - \Omega_0)^2}{\Omega_0} \right), \tag{8}
\]

\[
F_{area} = k_{\text{surface}} \left( \frac{k_B T}{2L_0^2} \frac{(S - S_0)^2}{S_0} \right) + \sum_{k \in 1, \ldots, N_t} \frac{k_{\text{shear}} k_B T (A_k - A_0)^2}{2L_0^2 A_0}, \tag{9}
\]

in which \( k_{\text{volume}}, k_{\text{surface}}, \) and \( k_{\text{shear}} \) are volume, surface, and local triangle area constants. \( \Omega, S, \) and \( A_0 \) are the volume, surface, and triangle area of the cell, while \( 2\Omega_0, S_0, \) and \( A_0 \) are the corresponding equilibrium values.

The force acting on vertex \( i \) is derived from \( \mathbf{f}_i = -\frac{\partial F(x_n)}{\partial x_i} \) and was calculated analytically.

The equilibrium quantities in Eqs. (5)–(9) are obtained from the initial shape and may differ per vertex and triangle. This ensures the absence of residual stresses in a similar fashion to the stress-free membrane model followed by Fedosov et al. [30]. The remaining simulation parameters, including those of the fluid, are shown in Table I. The density and viscosity ratio in the two poles of the sphere, similar to the stretching of an
RBC [28], yields a deviation of less than 0.08% from the initial radius.

Considering the low particle-Reynolds numbers used in this study (see Sec. III), the spheres are rendered near-rigid; however, due to the constitutive model, there are no residual stresses resulting from an inhomogeneous mesh; however, due to the constitutive model, there are no residual stresses resulting from an inhomogeneous mesh.

| TABLE II. Properties of spherical meshes, created by subdividing either a regular icosahedron or an octahedron. $N_v$ corresponds to the number of vertices, $N_t$ to the number of triangles, and the symbol $\sigma$ to the standard deviation of the quantity denoted in the subscript (as used in Sec. II B). The regular icosahedron produces more homogeneous meshes; however, due to the constitutive model, there are no residual stresses resulting from an inhomogeneous mesh.
| Initial shape | $N_v$ | $N_t$ | $\sigma_{A_0}/A_0$ | $\sigma_{L_1}/L_1$ | $\sigma_{\theta}/\theta_0$
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>icosahedron</td>
<td>162</td>
<td>320</td>
<td>8.5%</td>
<td>6.4%</td>
<td>14.3%</td>
</tr>
<tr>
<td>octahedron</td>
<td>258</td>
<td>512</td>
<td>23.9%</td>
<td>14.9%</td>
<td>39.0%</td>
</tr>
<tr>
<td>icosahedron</td>
<td>642</td>
<td>1280</td>
<td>8.6%</td>
<td>6.5%</td>
<td>15.9%</td>
</tr>
<tr>
<td>octahedron</td>
<td>1026</td>
<td>2048</td>
<td>24.2%</td>
<td>15%</td>
<td>40.9%</td>
</tr>
<tr>
<td>icosahedron</td>
<td>2562</td>
<td>5120</td>
<td>8.6%</td>
<td>6.5%</td>
<td>16.6%</td>
</tr>
</tbody>
</table>

The major advantage of the IBM is that the discretized fluid velocity is interpolated at the Lagrangian surface points and the computed forces are exerted to the closest Eulerian points according to

$$ f(X, t) = \sum_i F_i(t) \delta(X - x_i(t)), $$

where $\delta(X - x_i(t))$ is the discrete Dirac delta function. $f(X, t)$ is coupled to the LBM via the forcing term as described in Eq. (3).

Subsequently, the velocity of the membrane point $i$ is updated based on the local flow field and advected according to the Euler scheme

$$ x_i(t + \Delta t) = x_i(t) + u_i(t + \Delta t) \Delta t $$

or to the Adams-Bashforth scheme

$$ x_i(t + \Delta t) = x_i(t) + \left( \frac{1}{2} u_i(t + \Delta t) - \frac{1}{2} u_i(t) \right) \Delta t, $$

where

$$ u_i(t + \Delta t) = \sum_i u(X, t + \Delta t) \delta(X - x_i(t)) $$

The function $\delta(r)$ of Eqs. (10) and (13), used for the velocity interpolation and force spreading, is replaced by a product of 1D interpolation kernel functions $\phi_n$, where $n$ denotes the support of the kernel in all directions, as

$$ \delta(r) = \phi_2(x) \phi_2(y) \phi_2(z), $$

where $r = (x, y, z)$. In the present work, we make use of the following kernels:

$$ \phi_2(r) = \begin{cases} 1 - |r|, & |r| \leq 1, \\ 0, & 1 \leq |r|, \end{cases} $$

$$ \phi_3(r) = \begin{cases} \frac{1}{3} (1 + \sqrt{1 - 3r^2}), & |r| \leq 1, \\ \frac{1}{3} (5 - 3|r| - \sqrt{-2 + 6|r| - 3r^2}), & \frac{1}{2} \leq |r| \leq \frac{3}{2}, \\ 0, & \frac{3}{2} \leq |r|, \end{cases} $$

$$ \phi_4(r) = \begin{cases} \frac{1}{8} (3 - 2|r| + \sqrt{1 + 4|r| - 4r^2}), & |r| \leq 1, \\ \frac{1}{8} (5 - 2|r| - \sqrt{-7 + 12|r| - 4r^2}), & 1 \leq |r| \leq 2, \\ 0, & 2 \leq |r|. \end{cases} $$

The support of each kernel is shown in Fig. 1.

**FIG. 1.** Support functions for IBM kernels $\phi_2$, $\phi_3$, and $\phi_4$ [Eqs. (14), (15), and (16), respectively].
### Free parameters of the IB-LBM

The IBM comes with a number of free parameters. The most important are the interpolation kernel $\phi$, the number of surface vertices $N_v$, the lattice discretization $\Delta x$, the update scheme [Eqs. (11) and (12)], and the LBM relaxation time $\tau$. While it is implied that a finer spatial and mesh resolution, i.e., smaller $\Delta x$ and more $N_v$, respectively, would yield more accurate results, the computationally demanding case of dense suspensions can significantly benefit from identifying the limits and the artifacts of each parameter.

The interpolation kernel $\phi$ is the core of the IBM. It introduces an artificial length scale, effectively changing the thickness of the membrane. It is known that kernel $\phi_2$ [Eq. (14)] violates the translational invariance, and it has been found to introduce nonphysical oscillations $[10,13]$, yet $\phi_2$ is considered to capture the relevant physics and is still preferred due to its compact support (one $\Delta x$ in each direction), small numerical thickness, and reduced amount of computations $[6,17]$.

The number of surface vertices $N_v$ has been found to play only a minor role $[11,17]$, and a suggested mean vertex distance varies between 0.5 and 1.5$\Delta x$ $[17]$ (3D simulations) or 0.33$\Delta x$ $[6]$ (2D simulations) without compromising the impermeability of the particle membrane. The Euler update scheme is used more often in the literature, while Krüger $[17]$ argues that higher-order schemes, such as the Adams-Bashforth scheme, will not change the outcome of short simulations, yet it might provide additional accuracy for longer-time simulations. The effect of the LBM relaxation time $\tau$, on the other hand, has been found to be considerable on the IB-LBM simulations, in both simulations of capsules $[17]$ and when acting as velocity boundaries $[31]$. It is also worth noting that $\tau$ has a similarly considerable effect on bounce-back boundaries.

### III. Simulation Results

We consider three representative cases, accounting for the interactions of IBM membranes with the fluid and with other IBM membranes. First, we look into the behavior of the effective hydrodynamic radius $r_{\text{hyd}}$ of a sphere with radius $r$ in a sheared environment. Next, we investigate the interaction between two particles in a sheared environment. As our final case, two spheres are forced to collide as we examine the gap $h$ where lubrication forces break down.

All simulations correspond to the same system: a domain of $20r \times 20r \times 20r$ containing one or two spheres with a dimensional radius of 4 $\mu$m. The length and time scales are chosen for their relevance to red blood cell suspensions, which are of particular interest to our line of research, yet the results can be carried over to other systems following a similar dimensionless scaling. Dimensionless parameters used to characterize the system, such as Reynolds number and confinement, are fixed for all simulations in each benchmark. By using the same dimensional system, we highlight the differences imposed by choosing different IB-LBM parameters.

We use stiff spherical particles omitting additional interparticle forces, such as explicit lubrication or penetration correction, to capture the interactions arising purely from the IB-LBM. Finite-size effects were not considerable, i.e., they were less than 6% in all of the examined cases; see Appendix A.

### TABLE III. Default parameter set used for the simulations, unless stated otherwise.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice constant, $\Delta x$</td>
<td>1.0 $\mu$m</td>
</tr>
<tr>
<td>Radius of sphere, $r$</td>
<td>4.0 LU</td>
</tr>
<tr>
<td>Total number of vertices per sphere, $N_v$</td>
<td>258</td>
</tr>
<tr>
<td>Relaxation time, $\tau$</td>
<td>1.0</td>
</tr>
<tr>
<td>IBM kernel, $\phi_k$</td>
<td>$\phi_4$</td>
</tr>
<tr>
<td>IBM update scheme</td>
<td>Euler</td>
</tr>
</tbody>
</table>

The default parameter set is shown in Table III, with each figure that follows explicitly denoting the parameters that were varied. Note that when the radius of the particle is varied, what actually changes is the lattice constant $\Delta x$, resulting in a different particle radius in lattice units. In other words, all simulations have the same dimensional radius, yet they differ in lattice resolution. In the cases in which the LBM relaxation parameter $\tau$ is changed, the time step changes according to the diffusive scaling relation $\Delta t = \frac{\tau_{LB}}{\Delta x^2}$, where $\tau_{LB}$ is the lattice viscosity. The parameters of the membrane model presented in Table I have been scaled accordingly to correspond to the same dimensional system. Results are presented in two forms, dimensional and dimensionless, always denoting the unit: $\mu$m for dimensional and LU for lattice units.

#### A. Hydrodynamic radius of a sphere

Einstein’s well-known relation $v_{\text{rel}} = 1 + 2.5\phi V$ connecting the relative apparent viscosity $v_{\text{rel}}$ of a dilute suspension with the volume fraction $\phi V$ is a convenient way to measure the effective hydrodynamic radius of a sphere by measuring its volume. The effective hydrodynamic radius of a sphere is then measured as

$$r_{\text{hyd}} = \sqrt{\frac{3}{4\pi}} \phi V, \quad (17)$$

where $V$ is the volume of the domain, equal to $(20r)^3$. The volume fraction is $\phi V = 0.0525\%$ and is well within the limits of Einstein’s relation between volume fraction and apparent viscosity.

The hydrodynamic radius is a measure of the hydrodynamic size of the particle as felt by the fluid and the contribution of the particle to the viscosity of the suspension. It is not intended to be used as a recalibration parameter.

The imposed radius, the hydrodynamic radius, and their difference $\Delta r_{\text{hyd}}$ are shown in Fig. 2(a). The maximum extent of $r_{\text{hyd}}$ is defined by the support of the IBM kernel. For $\phi_4$ this is $\pm 2$ LU. Parameters such as the radius $r$ of the sphere, the relaxation time $\tau$, and the surface density of the vertices, $N_v/S_{LU}$, where $S_{LU}$ is the surface of the sphere, control the actual extent of the radius.

The sphere is placed between two plates in a shear-flow environment, as depicted in Fig. 2(b). The fluid is initialized at rest. From the two parallel plates, only the top one is moving and the bottom measures the shear stress of the suspension via the momentum-exchange method $[32]$. The location of the bottom boundary wall is considered to be halfway between the bounce-back node and the first fluid node, since $\tau = 1.0$ $[33]$. 

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To verify this approach, we perform fluid-only simulations and obtain a relative viscosity of $\nu_{\text{rel}} = 0.038$.

**Results**

The effective hydrodynamic radius $r_{\text{hyd}}$ is measured as the time average of $r_{\text{hyd}}(t)$ from $\gamma t = 10$ to $25$, as shown in Fig. 3(a), while the error bars in the plots are defined as the standard deviation during this time period.

The hydrodynamic radii for dimensional and dimensionless units are shown in Figs. 3(a) and 3(b), respectively. Coarser spatial resolutions, where the radius of the sphere is expressed with fewer lattice units, result in an increased $r_{\text{hyd}}$. For example, a sphere radius of 8 LU appears increased by only $\sim 10\%$, while when $r = 2.7$ LU its increase is $\sim 35\%$, indicating the latter as a coarser representation.

Figures 3(b) and 3(c) contain the same data, yet they are plotted against different quantities. The spatial resolution dominates the increase, which, in absolute numbers, seems unaffected by the vertex density [inset of Fig. 3(d)]. For the cases $r = 4.0, 5.0,$ and 8.0 LU, Fig. 3(c) shows that $\Delta r_{\text{hyd}}$ is small for $N_x/S_{LU} < \sim 2$ (and seemingly constant for $r = 8.0$ LU), and for $N_x/S_{LU} > \sim 2$ it jumps to a higher value. This threshold is more visible for kernels with smaller support, such as $\phi_2$ and $\phi_3$ [Fig. 3(d)], while the increase in $r_{\text{hyd}}$ for adequate mesh resolutions is independent of the IBM kernel used. The increase for underresolved meshes is almost half of that for the finer mesh resolutions, which may be due to the fluid penetrating the membrane. For the lower resolutions, this highlights that being closer to the input radius is not the desired outcome, but a consequence of the underresolved mesh. IBM kernel $\phi_4$ is more robust in low mesh resolutions, counteracting what in $\phi_2$ and $\phi_3$ appears as membrane permeability. $\phi_4$ has twice the support of $\phi_2$, thus extending the reach of each vertex, allowing for meshes with fewer surface vertices to appear coherent.

It is also worth noting that the use of a higher-order scheme, such as the Adams-Bashforth scheme [Eq. (12)], had no impact on the results we obtained (data not shown).

**B. Interaction between nearby membranes**

1. Two spheres in shear flow

One important benchmark for transport studies is the interaction of two spheres in a simple shear-flow environment. Analytical solutions for this system have been derived by Batchelor and Green [19] for systems without boundaries and inertia. Depending on the initial distance of the two spheres, their trajectories can either extend to infinity or be finite, characterized as open or closed trajectories, respectively. In these open trajectories, two smooth spheres return to their original streamlines after a collision, where potential asymmetries between pre- and postcollisional positions lead to shear-induced dispersion [20,21]. In bounded cases of Couette flow, a neutrally buoyant sphere migrates toward the center of the domain [34], and the origin of this migration lies in the interaction of the force dipole generated by the particle and its image in the wall [35].

We place two identical spheres in a linear shear-flow domain of size $(20r \times 20r \times 20r)$ and apply a shear rate of $\gamma = 132.8/s$, resulting in a particle-Reynolds number of $Re_p = 0.005$, using the input radius. The initial distance between the two spheres is $\Delta X_0, \Delta Y_0, \Delta Z_0 = (10r, 1.5r, 0)$, where the $y$ direction is the shear-gradient direction. The setup is shown in Fig. 4.

We are interested in the collision distance in the $y$ direction, $\Delta Y_{\text{max}} = \Delta Y_{\text{inter}}$, which occurs when $\Delta X = 0$, and from that we define the interaction radius $r_{\text{inter}} = \Delta Y_{\text{max}}/2$. Under the assumption of smooth spheres and low $Re_p$, two spheres of equal size pass very close to each other, so that $\Delta Y_{\text{max}} \to 2r$, while having symmetric pre- and postcollisional trajectories [19]. The increase in the interaction radius is measured as $\Delta r_{\text{inter}} = r_{\text{inter}} - r$. The increase $\Delta r_{\text{inter}}$ is not a particle property and is used as a reference to study deviations that may vary between simulations.

2. Results

Figure 5 shows the parametric plots of $\Delta Y/r$ versus $\Delta X/r$ for varying mesh resolutions and $\tau = 1.5$. The migration of the spheres toward the center of the domain can be distinguished before and after the collision.

As shown in Figs. 6(a), 6(b) and 6(c), the interaction radius $r_{\text{inter}}$ is systematically larger than the hydrodynamic radius $r_{\text{hyd}}$ of the previous section. This result excludes the use of $r_{\text{hyd}}$ as a parameter that can be used to recalibrate $r$ in order to obtain more accurate results. With respect to mesh resolution, $\Delta r_{\text{inter}}$ levels off about $\sim 1$ vertex per LU for adequately resolved meshes [inset of Fig. 6(a)], contrary to $\Delta r_{\text{hyd}}$.

In this benchmark, choosing an interpolation kernel $\phi_n$ with a larger support increases the interaction radius while preserving the discrepancies between the underresolved and adequately resolved meshes [see Fig. 6(c)]. Increasing the relaxation time $\tau$ leads to decreasing $r_{\text{inter}}$ [Fig. 6(d)]. A similar behavior was also observed by Nguyen and Ladd [22] for the momentum-exchange algorithm [32,36]. In this view, the IBM behaves similarly to the LBM’s bounce-back boundaries, where the position of the boundary depends on the relaxation time $\tau$ [33].

One cannot help but notice the decrease in $\Delta Y/r$ before and after the collision in Fig. 5, which increases as $N_x$ increase.
This shift corresponds to the migration of neutrally buoyant spherical particles in a Couette flow toward the center of the domain, and it depends on the ratio of the diameter of the particle to the distance between the walls and on the particle-Reynolds number [34]. Kromkamp et al. [23] have also noticed an increase in migration with increasing Re_p in their simulations. Our results, however, point to inconsistent behavior regarding this migration. The particle Re used is relatively small (∼0.005) and the domain sufficiently large for this to be a finite-size effect [37]. To quantify this behavior, we define the precollision shift as ΔY_{shift} ≡ min(ΔY_{Ax}/r<0) − ΔY_0.

Figure 7(a) suggests that the cases that appeared to be underresolved in the previous cases do not migrate toward the center of the vessel, while migration increases as the vertex density increases. Below the threshold of two vertices per LU^2 there is no migration, suggesting that fluid penetration significantly affects the transport of vesicles in bounded geometries. This is more obvious when using φ_2, which does not produce any migration, even in the finer mesh resolutions.

The migration is independent of the relaxation time τ [Fig. 7(c)], while using the Adams-Bashforth scheme produced the same results, thus having no effect in the course of the simulation (data not shown).

3. Lubrication forces between two spheres

Finally, we study the lubrication interaction of two spheres. Since the IBM is based on interpolation, the hydrodynamic
interaction of two particles whose surface vertices are close can be accurately resolved up to a certain limit, defined mainly by the support of the kernel and the vertex surface density. Vertices that are close to each other exert force to nearby nodes and interpolate similar velocities, inducing a form of correlation between them. In addition to the overlapping IBM kernels, the fluid flow in their gap cannot be accurately resolved up to a certain limit, defined mainly by the support of the kernel and the vertex surface density.

In this benchmark, we study approaching spheres and lubrication torque. For particles coupled with the momentum-exchange algorithm (MEA), Nguyen and Ladd [22], based on analytical results of Jeffrey and Onishi [38], proposed a correction for the lubrication force between two spheres with radii $r_1$ and $r_2$ when they are closer than a cutoff distance $h_N$ (assuming forces to be independent of gap, for gaps smaller than $h_N$):

$$F_{\text{lub}} = \frac{6\rho v}{r_1 \cdot r_2} \left( \frac{1}{h} - \frac{1}{h_N} \right) U_{12} \cdot \hat{R}_{12}, \quad h < h_N,$$

$$= 0, \quad h \geq h_N. \quad (18)$$

$U_{12} = U_1 - U_2$ refers to the velocity difference between the two spheres, $h = |\mathbf{R}_{12} - r_1 - r_2|$ to the gap between the two surfaces, and $\hat{R}_{12} = \mathbf{R}_{12}/|\mathbf{R}_{12}|$ is the unit vector connecting the centers of the two spheres. Equation (18) essentially shows that $F_{\text{lub}} \propto U_{12}^{\text{normal}}/h$ in the limit of $h \to 0$.

The purpose of these simulations is not to propose a lubrication correction scheme for the IBM, but rather to indicate the range in which lubrication is accurately resolved for the IBM surfaces. We use the domain of Sec. III B 1 with $\gamma = 0/s$ and dimensions $(20r \times 20r \times 20r)$ to measure the distance at which the lubrication breaks down. The two spheres are separated by an initial distance of $(\Delta X_0, \Delta Y_0, \Delta Z_0) = (10r, 0, 0)$.

In the scheme we are using, we cannot impose velocity and measure force, as is commonly practiced in these studies [22,24]. Instead, we apply a constant and opposite force of $F_0 = 125 \text{ pN}$ in the $x$ direction on each sphere, and we measure their relative distance. There are several variants of the IBM to simulate rigid bodies, however this would imply using a different scheme, and comparisons with the earlier results would be invalid.

This force may introduce an artificial density difference between the inner and the outer fluid, yet due to the simplicity of the system, potential side effects similar to [24] are considered to be minor. However, it is believed that they would not change the outcome considerably. Due to anisotropies in the discretization of the membrane, spheres that are forced may roll over each other and diverge from the head-on collision. To ensure that this will not happen, an additional spring force is considered, keeping the centers of the two spheres aligned with the direction of the force. The force is defined as $F_{\text{corr}} = (0, -F_0 \frac{T_{\mu m}}{1 \mu m}, -F_0 (Z-Z_0))$.

### 4. Results

The quantity we are interested in is the gap $h$ between the two spheres, and in particular $h_{\text{fail}}$, the point where lubrication forces break down (for a description of the definition of $h_{\text{fail}}$, please see Appendix C). Figure 8(b) shows the evolution of $h$ with respect to time. A point is evident, in which the course of the trajectories changes, indicating that the lubrication force is not accurately resolved.

Parameter sets in which spheres have a small effective radius take substantially longer to reach $h_{\text{fail}}$. In our case, these simulations terminate within the designated simulation time before this point. Cases with larger surface density break down at larger distances [see Fig. 9(a)], while $h_{\text{fail}}$ seems to be independent of $\tau$, as shown in Fig. 9(b). Deformations of the spheres were negligible. In this benchmark, the use of the Adams-Bashforth scheme had no impact on the results we obtained (data not shown).

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**FIG. 4.** Schematic for the case described in Sec. III B 1. Two spheres are positioned in a shear-flow environment at rest, and the relative distance between their centers is measured.

**FIG. 5.** Flow trajectories for two interacting spheres in shear flow. The number of vertices range from 162 to 1026 for a sphere of 4 LU. ● denotes the collision distance $\Delta Y_{\text{max}}$ and ■ denotes the "precollision shift" $\Delta Y_{\text{shift}}$. Spheres with high resolution ($N_v = 1026$) migrate toward the center of the domain.
FIG. 6. (a) Dimensional interaction radius vs imposed radius. Transparent symbols correspond to the values measured in Sec. III A. Finer resolutions mitigate the increase in the effective interaction (and hydrodynamic) radius of a sphere. Inset: same data where the increase $\Delta r_{\text{hyd}}$ is now measured in lattice units. (b) Increase in dimensional interaction radius, $\Delta r_{\text{inter}}$, in lattice units with respect to the vertex surface density $N_v/S_{LU}$. Transparent symbols correspond to the values measured in Sec. III A. (c) Increase in interaction radius, $\Delta r_{\text{inter}}$, with respect to the interpolation kernel $\phi_n$, for $r = 4.0 LU$. Transparent symbols correspond to the values measured in Sec. III A. Interpolation kernels with larger support increase the interaction radius, while $N_v = 162$ and 258 still appear to result in lower $r_{\text{inter}}$ due to the low surface resolution. (d) Increase in interaction radius, $\Delta r_{\text{inter}}$, with respect to the relaxation time $\tau$, for $r = 4.0 LU$. Increasing $\tau$ decreased the interaction radius $r_{\text{inter}}$.

FIG. 7. Normalized precollision shift, $\Delta Y_{\text{shift}}/r$: (a) with respect to the vertex surface density $N_v/S_{LU}$; (b) with respect to the interpolation kernel $\phi_n$; and (c) with respect to the relaxation time $\tau$. 

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FIG. 8. (a) Schematic for the case described in Sec. III B 3. Two spheres are positioned in a resting fluid and forced toward each other. Their relative positions and gap are measured. (b) Gap $h$ in units of radius, vs dimensionless time, for varying lattice spacings $\Delta x$. The symbol $\times$ identifies $h_{\text{fail}}$, the gap in which the lubrication forces fail. In setups with larger effective radii (namely larger $\Delta x$), their failure occurs in larger gaps $h/r$, while they need more time to reach to the same gap.

IV. DISCUSSION

In this work, we present a parametric study for the combined IB-LBM method applied in simulations of one and two suspended particles. We have studied the sensitivity of the simulation results to the lattice constant $\Delta x$, the number of vertices $N_v$, the interpolation kernel $\phi$, and the LBM relaxation time $\tau$. Computational complexity increases as $\sim f^5$ with a spatial refinement factor $f$ for the LBM subsystem, and $\sim f^2$ for the membrane model from the time step alone without remeshing, and thus the urge to reduce the resolution is high. However, care has to be taken in the choice of parameters since the accuracy of the computations is drastically reduced if mechanical and hydrodynamical interactions are insufficiently resolved. We hope that the presented benchmarks will help other users of the methods to choose the parameters according to the requirements of their applications.

An important conclusion we obtained from the first two benchmarks is that there exists a difference between the radius “felt” by the fluid (i.e., via the stress exerted and measured by $r_{\text{hyd}}$) and the radius “felt” by hydrodynamically interacting spheres. This implies that a consistent effective radius, which could account for the increase, does not exist. Neither $r_{\text{hyd}}$ nor $r_{\text{inter}}$ can be used to recalibrate the radius of the suspended particle.

In the three benchmarks we have performed, we found that each parameter has its distinct effect on the interaction of the membrane with the fluid and other membranes. Spatial resolution strongly determines the extent of the effective hydrodynamic and lubrication radii of the particle, which, in contrast, are influenced less by membrane-vortex density. In

FIG. 9. (a) Failing gap $h_{\text{fail}}$ with respect to vertex surface density. Transparent symbols correspond to $2 \times r_{\text{inter}}$. (b) Failing gap $h_{\text{fail}}$ with respect to $\tau$. 

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our simulations we found that mesh resolutions of fewer than two vertices per LU$^2$ will lead to potential fluid penetration. The effects of underresolved meshes are even more profound for IBM kernels with a smaller support, such as $\phi_2$. In the lubrication limit, i.e., for small gaps between the particles, high membrane-vertex density and larger kernels lead to an overestimation of the hydrodynamic interactions. A consistent correction such as that proposed by Nguyen and Ladd [22] for particles coupled to the LBM fluid using the momentum-exchange method would need to take all these effects into account and is not known to date.

Underresolved meshes were also unsuccessful in reproducing the migration of a sphere toward the center of the vessel in a bounded shear flow, thus failing to capture essential physics. This was observed in all cases in which kernel $\phi_2$ was used, raising some concerns about whether it captures the relevant physics at all. Using $\phi_4$ leads to a more accurate reproduction of the particle migration, highlighting again the importance of mesh resolution. It produces, however, larger effective hydrodynamic radii and fails to resolve the hydrodynamic interaction of two particles in the lubrication limit.

Concluding on a universal set of parameters is not straightforward, and one must differentiate between dilute and dense suspensions. In dilute suspensions, where the mean distance between particles is relatively large, the finer resolutions produce a more accurate response. Interpolation kernel $\phi_2$, when the mesh is not properly resolved, appears to be “leaky,” in contrast to $\phi_4$, which is more robust with respect to the mesh resolution. A particle radius of $r = 4$ LU seems to be sufficient, while the mesh resolution is suggested to be kept above at least 2 points/LU$^2$ to reproduce the relevant physics. Relaxation time $\tau$ does not significantly affect the validity of the method, and since it defines the reach of bounce-back nodes and the time step of the LBM part, it depends on the specific problem. A value of $\tau = 1$ is a good tradeoff between accuracy and efficiency for the LBM.

The strength of $\phi_4$ in dilute suspensions is a weakness for the dense case, where the mean interparticle distances are small. Interpolation kernel $\phi_4$ has a notable numerical membrane thickness, which leads to the breakdown of the lubrication forces in larger gaps. This could be compensated for by adding an extra lubrication-correction force similar to [22,24], yet this exceeds the scope of this paper. In these cases, $\phi_2$ with the small numerical thickness can be combined with an adequately resolved mesh to avoid lubrication breakdown. However, if walls are present it is open to question whether the wall-particle interaction would be accurately captured.

Updating the position with the Adams-Bashforth scheme did not yield any differences compared to the Euler scheme, which is simpler and faster and thus preferred over more complex schemes. This was to be expected since LBGK is first-order accurate in time. Higher-order schemes might produce different results.

The number of free parameters is large, and an exhaustive study in three dimensions is challenging, given the low particle-Reynolds numbers and the domain sizes. We explored a parameter space sufficiently large to make the statements above, however further analysis is necessary to identify and understand the various side effects of a combined LBM-IBM scheme. Again, we would like to point out that it is important to perform a series of relevant benchmarks prior to a study in order to validate the choice of parameters.

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FIG. 10. Finite-size analysis of the cases presented in Sec. III. (a) The case of measuring the hydrodynamic radius from the suspension viscosity. Evolution of the hydrodynamic radius $r_{\text{hyd}}$, as calculated from Eq. (17) with respect to the dimensionless time $\dot{\gamma}t$. The different equilibration times are noticed for the two domain sizes. The values obtained differ by $\sim 2.7\%$. (b) The case of two spheres colliding in shear flow. Parametric plot of relative distances in the $x$ and $y$ directions for the two different domain sizes. The values for the calculated $\Delta X/r$ between the two domains differ at $\sim 0.5\%$ of the particle radius. (c) Case of head-on collision of two forced spheres. Evolution of the gap size normalized by the radius for the two different domain sizes. The difference between results from the two domains is within $\sim 6\%$.
APPENDIX A: FINITE-SIZE EFFECTS

A finite-size analysis was performed for the results presented in this paper. We compared results for all three cases between the domain used \((20r \times 20r \times 20r)\), where \(r\) is the radius of the sphere, and by doubling the size of the domain in each direction, namely \((40r \times 40r \times 40r)\). Results are presented in Fig. 10. In this analysis, we chose the coarse sphere representation, \(r = 2.7\) LU, with \(N_v = 258\) vertices, \(\tau = 1.0\), and the IBM interpolation kernel \(\phi_3\). The results obtained, as shown in Fig. 10, are qualitatively and quantitatively very similar. Since the “larger” domain of \(40r \times 40r \times 40r\) is eight times more demanding computationally (in terms of time and storage) than the “smaller” domain, the latter was chosen for the simulations.

To conclude, the finite-size analysis produced adequately similar results to justify the use of the smaller domain.

APPENDIX B: DEPARTURE FROM THE SPHERICAL SHAPE

In this appendix, we track the deformation of spheres as they collide in shear flow, as presented in Sec. III B 1. The metric used for the deformation is defined as \(D = (\max \{r_i\} - \min \{r_i\})/r\), with \(r_i = |\mathbf{R}_i - \frac{1}{N_v} \sum_{j=1}^{N_v} \mathbf{R}_j|\) being the distance of vertex \(i\) from the center of a sphere with \(N_v\) vertices. It is a very sensitive measure and can sense local divergences.

Figures 11(a) and 11(b) track this deformation with respect to the relative distance in the \(x\) direction, \(\Delta X/r\). These two cases represent one case in which the postcollision migration is negligible [Fig. 11(a)] and one in which it is significant [Fig. 11(b)]. In both of the samples, the deformation \(D\) is less than 0.8\%, yielding a maximum difference in the radii of the vertices of 0.032 LU. This is considered to be only a minor departure from the spherical shape.

To conclude, no significant deviation from the spherical shape was observed for the cases considered, rendering the objects we used spherical.

APPENDIX C: METRIC FOR LUBRICATION FAILURE

Defining the gap \(h_{\text{fail}}\), in which the lubrications fail, is not a straightforward task. The radii of the spheres are not exact, and methods other than using Eq. (18) have to be employed. We have noticed in the log-log plot of the gap versus time [like Fig. 8(b)] that after failure, it becomes linear in log-log space with an exponent \(n\), which is \(-1 < n < 0\). The exponent before can be seen as less than \(-1\), hence if multiplied by time \(t\), quantity \(ht\) can be used to distinguish the two regimes, as shown in Fig. 12(a).

By visual inspection, we verified that the gaps \(h_{\text{fail}}\) have been identified correctly in the cases presented.

FIG. 11. Departure of the two particles from the spherical shape for the interaction of two spheres in shear flow. Two cases are sampled: (a) one with a minor postcollision displacement and (b) one with a measurable postcollision displacement. The parameters of each simulation are mentioned in the title of each plot, and the inset images depict the relative positions of the two spheres. The deviations are considered to be minor.

FIG. 12. Quantity \(ht/r\), used to identify \(h_{\text{fail}}\). The symbol \(\times\) identifies \(h_{\text{fail}}\) as the local minimum of this quantity, while \(\circ\) identifies the first local maximum.


[37] The dimensions of the system were doubled and yielded the same effects, while simulating each sphere individually also produced a migration toward the center (data not shown).