Coupling fully resolved light particles with the Lattice Boltzmann method on adaptively refined grids

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Abstract

The simulation of geometrically resolved rigid particles in a fluid relies on coupling algorithms to transfer momentum both ways between the particles and the fluid. In this article, the fluid flow is modeled with a parallel Lattice Boltzmann method using adaptive grid refinement to improve numerical efficiency. The coupling with the particles is realized with the momentum exchange method. When implemented in plain form, instabilities may arise in the coupling when the particles are lighter than the fluid. The algorithm can be stabilized with a virtual mass correction specifically developed for the Lattice Boltzmann method. The method is analyzed for a wide set of physically relevant regimes, varying independently the body-to-fluid density ratio and the relative magnitude of inertial and viscous effects. These studies of a single rising particle exhibit periodic regimes of particle motion as well as chaotic behavior, as previously reported in the literature. The new method is carefully compared with available experimental and numerical results. This serves to validate the presented new coupled Lattice Boltzmann method and additionally it leads to new physical insight for some of the parameter settings.

KEYWORDS:
Lattice Boltzmann Method; Direct Numerical Simulation; Adaptive Grid Refinement; Explicit Coupling; Light Sphere

1 | INTRODUCTION

Light particles, here understood as particles with a solid-to-fluid density ratio \( \rho_p = \rho_f / \rho_0 < 1 \), appear in various applications and situations. During ascension in an otherwise resting fluid they exhibit a multitude of movement patterns often strongly deviating from straight paths. This depends on shape, density ratio, and surrounding fluid properties. As a matter of fact, strictly straight paths only occur in a comparatively small parameter range. This makes way to consider the implications of such non-regular paths in practical settings. As an environmental problem, floatsam in the form of microplastics with a density slightly lower than water may harm the biosphere in oceans and lakes. Here the density ratio ranges from \( \rho_p \approx 0.9 \) for polypropylene to \( \rho_p \approx 0.01 \) in the case of expanded polystyrene. Furthermore, in a natural setting, rising bubbles and particles in oceans support the formation of warmer regions with stronger temperature gradients. Facilitating the dispersion of fluid and matter, the turbulent structures induced by moving bubbles of low density ratios in a mixture is also of interest in engineering applications. Two examples are fuel sprays in combustion engines and bubbly flows in industrial reaction catalysis. In aerodynamics the effects are observed for meteorology balloons and in the context of autorotation of individual objects.
Above examples typically involve a huge number of particles, whereas even the movement of a single spherical particle exhibits complex behaviors. A light, spherical body submerged in water under the sole influence of gravity may either rise in a straight line, move obliquely, enter a regular or rather chaotic zig-zagging movement. As reported by Jenny et al.\textsuperscript{15} this depends on the density ratio $\pi_p$ and the Galileo number $Ga$, which describes the ratio between buoyant and viscous forces. They used numerical simulation to study the particle paths, varying these two parameters. In the following, Veldhuis & Biesheuvel\textsuperscript{10}, Horowitz & Williamson\textsuperscript{17} and Ostmann, Chaves & Brucker\textsuperscript{18}, among others, performed laboratory experiments to obtain physical comparison results. To address the found contradictions, Zhou & Dušek\textsuperscript{19} and Auguste & Magnaudet\textsuperscript{20} performed an extensive set of detailed numerical simulations. Albeit very efficient for such specific setups, these recent simulation approaches are usually not extensible to multiple particles or arbitrary domains due to the usage of spectral methods, making them only suitable for a single freely moving sphere.

Such restrictions are not present for other methods in computational fluid dynamics (CFD), such as finite volume methods\textsuperscript{21-23} or the lattice Boltzmann method\textsuperscript{24-26} (LBM). Many of the previously mentioned scenarios involving bubbly flows can be approximated by modeling those submerged small bubbles as rigid spheres in a fluid due to their low Eötvös number\textsuperscript{27}. This enables the usage of a Lagrangian description for the solid phase by employing discrete particle simulation. In combination with fluid-particle coupling that enables geometrically fully resolved simulations of the flow around the particle and the fluid-solid interactions, predictive studies of a large variety of particulate systems become possible\textsuperscript{28-30}. In this work, we focus on the LBM which is a relatively recent Eulerian computational method to simulate fluids. The LBM is well suited for large scale simulations and massively parallel execution\textsuperscript{31-33}.

The fully coupled interaction between the solid Lagrangian and the fluid Eulerian phase is achieved by the momentum exchange method (\textit{MEM-LBM})\textsuperscript{34,35}. However, the \textit{MEM-LBM} on its own is only partially applicable for simulations of light particles, as intended in the present work. It is known to suffer from instabilities when density ratios approach zero. The stability condition of the original coupling by Ladd et al.\textsuperscript{36} was given as $\pi_p d_p / \Delta x > 20$, where $d_p / \Delta x$ is the numerical resolution in terms of cells per particle diameter. With the improvements by Aidun et al.\textsuperscript{37}, density ratios close to one could be realized.

This issue of numerical instability at those circumstances is not restricted to the \textit{MEM-LBM} and reported for many CFD methods that apply an explicit fluid-particle coupling. For the popular immersed boundary method\textsuperscript{38} (IBM), e.g., the lower bound initially resided at $\pi_p = 1.2$. Improvements to the imposition of boundary conditions on the interface and an additional integration step for the artificial flow field inside the particles allowed stable results at $\pi_p > 0.3$\textsuperscript{39}. To gain a fully stable solution at arbitrary density ratios, much more costly implicit schemes were proposed\textsuperscript{40-42}.

The reason for the instabilities in explicit coupling schemes is attributed to the particles’ mass being exceeded by its so-called added mass, i.e. the fluid attached to the moving particle. In an explicit coupling scenario, this mass cannot be properly accounted for, which results in excessive accelerations on startup that lead to oscillations\textsuperscript{43}. In an effort to stabilize explicit schemes at density ratios as low as $\pi_p = 0.001$, Schwarz et al. investigated the cause of stability issues in the IBM\textsuperscript{44}. By introducing an auxiliary virtual force and a virtually increased mass of purely numerical nature to the particle, stable simulations of light particles could be obtained. This scheme was termed the “virtual mass approach” by the authors.

In this paper, we aim to improve the existing \textit{MEM-LBM} and extend it to simulations of particles with very low density ratios. To this end, we follow and improve the approach by Schwarz et al., resulting in a \textit{MEM-LBM} enhanced by virtual mass (\textit{VM-MEM-LBM}). This will allow for predictive numerical studies of such setups. As an illustrative example and to demonstrate the applicability of our approach, we investigate the movement of a single rising sphere in an unbounded domain. In an effort to validate existing results from literature, demonstrate the capabilities of the \textit{VM-MEM-LBM} and enabling a scalable simulation of submerged light spheres, we apply the LBM to this problem. To our best knowledge, our article is the first to apply the LBM in a wide range of parameter settings of this situation.

Improving the efficiency of these simulations, an adaptive grid refinement technique is employed. Since domains with a height in the order of 100 times of the sphere diameter are necessary, many regions of the fluid remain stale during the motion of the sphere, requiring only coarse resolutions. On the other hand, increasing turbulences and strong velocity gradients especially at the fluid-solid interface require a high resolution to yield satisfying results. Thus, a grid, which locally adapts its spacing, is desirable.

The paper is structured as follows. In Section\textsuperscript{2} the \textit{MEM-LBM} as used for the simulations throughout this paper is outlined. Section\textsuperscript{3} starts with a numerical study to investigate and discuss the lower density ratio limits of the \textit{MEM-LBM}. Next, this method is enhanced by the virtual mass approach, resulting in the \textit{VM-MEM-LBM}. Efficiency improvements by employing adaptive grid refinement and criteria for determining the need of a change in resolution are explained in Section\textsuperscript{4}. Section\textsuperscript{5}
presents an extensive study of the movement trajectories and vortices of rising spheres to demonstrate the practical use of MEM-LBM and VM-MEM-LBM. We conclude with a summary in Section 6.

2 | NUMERICAL METHOD

The here employed CFD method is based on the recently developed approach presented and validated in Ref. 46. For completeness, we outline the main aspects of the fluid flow simulation and the fluid-particle coupling in the following and refer to this work for a more detailed description. All presented methods can be found in the open-source repository of the WALBERLA framework.

2.1 | Lattice Boltzmann Method

The lattice Boltzmann method (LBM) is based on an Eulerian representation of the fluid field by mesoscopic kinetic equations, that fulfill the macroscopic Navier-Stokes equations. It computes the temporal evolution of particle distribution functions (PDFs) \( f_q \) in the cells of a Cartesian lattice using a discrete solution of the Boltzmann equation. The LBM is commonly described using the \( \text{D}d\text{Q}q \) notation with \( d \) spatial dimensions and \( q \) discrete velocities \( c_q \). A common choice for three dimensional simulations is \( \text{D}3\text{Q}19 \) which will be employed throughout this paper.

Being an explicit numerical scheme in time, the equation to advance the PDFs of a cell \( x \) by one time step of size \( \Delta t \) is given by

\[
f_q(x + c_q \Delta t, t + \Delta t) = f_q(x, t) - C_q(f_1(x, t), ..., f_{19}(x, t)),
\]

where \( C \) corresponds to a general collision operator. It is applied during the collision step, i.e. the right part of the equation, to update the local PDFs in each cell \( x \) inside the domain. The left part denotes the streaming step of the LBM, which constitutes distribution of the post-collision PDFs \( f_q(x, t) \) to the neighboring cells.

The local macroscopic fluid density \( \rho_f \) and velocity \( u_f \) are given as moments of the distribution functions,

\[
\rho_f(x, t) = \sum_q f_q(x, t), \quad \rho_b u_f(x, t) = \sum_q f_q(x, t)c_q,
\]

where \( \rho_0 \) is a constant average density, that is introduced to reduce inherent compressibility effects.

In LBM, quantities are commonly formulated in so-called lattice units, such that the cell size \( \Delta x = 1 \), time step size \( \Delta t = 1 \) and \( \rho_0 = 1 \).

In the multiple-relaxation-time (MRT) formulation, the collision operator \( C \) is written using a diagonal relaxation matrix \( S \), containing the relaxation factors, and a corresponding matrix \( M \), which linearly transforms the distribution functions to the moment space, where the collision is carried out. The collision operator is thus given as

\[
C = M^{-1}SM.
\]

In particular, we here employ the specific MRT model from Ref. 46 which uses the transformation matrix \( M \) given in Ref. 51 and the relaxation matrix

\[
S = \text{diag} \left( 0, 0, 0, 0, s_b, s_b, s_b, s_b, s_b, s_b, s_b, s_b, s_b, s_b, s_b, s_b, s_b, s_b, s_b, s_b \right).
\]

Via its three parameters, it allows for explicit control over the kinematic fluid viscosity \( \nu_f \) and the bulk viscosity \( \nu_b \), given as

\[
\nu_f = c_s^2 \Delta t \left( \frac{1}{s_v} - \frac{1}{2} \right), \quad \nu_b = \frac{2}{3} c_s^2 \Delta t \left( \frac{1}{s_v} - \frac{1}{2} \right),
\]

with the lattice speed of sound \( c_s \), and provides an accurate representation of boundaries. Parameterization can conveniently be done by introducing the so-called “magic” parameter \( \Lambda \) which we set to \( 3/16 \), and a bulk factor \( \Lambda_b \).

\[
\Lambda = \left( \frac{1}{s_v} - \frac{1}{2} \right) \left( \frac{1}{s_v} - \frac{1}{2} \right), \quad \Lambda_b = \left( \frac{1}{s_v} - \frac{1}{2} \right) \left( \frac{1}{s_v} - \frac{1}{2} \right).
\]

Choosing \( \Lambda_b = 1 \) results in the two-relaxation-time (TRT) collision operator. Unless stated otherwise, we employ \( \Lambda_b = 100 \).
Throughout the paper, we consistently make use of the commonly applied lattice unit system, given by the cell size $\Delta x = 1$, the time step size $\Delta t = 1$, $c_s = 1/\sqrt{3}$, and $\rho_0 = 1$.

2.2 Rigid Particle Motion

The Lagrangian dynamics of a spherical rigid particle is governed by the temporal evolution of its position $x_p(t)$, translational velocity $u_p(t)$, and angular velocity $\omega_p(t)$, and is described by

$$\frac{dx_p}{dt} = u_p, \quad \frac{du_p}{dt} = F_p, \quad \frac{d\omega_p}{dt} = T_p,$$

(7a)

(7b)

(7c)

where $m_p = \rho_p V_p$ is the particle’s mass, with the particle density $\rho_p$ and its volume $V_p$, and $I_p$ corresponds to its moment of inertia. Gravitation and buoyancy contributions are given as $F_p^g = (\rho_p - \rho_f)g V_p$, with the gravitational acceleration $g$. Together with the fluid-particle interaction force $F_p^{\text{hyd}}$, they are the total force acting on the particle, $F_p = F_p^g + F_p^{\text{hyd}}$. Accordingly, the particle’s torque is $T_p = T_p^{\text{hyd}}$. Temporal integration of Equations (7a) to (7c) is achieved by explicit time stepping using a Velocity-Verlet scheme. The explicit update formulas are expressed as

$$x_p(t + \Delta t) = x_p(t) + \Delta t u_p(t) + \frac{\Delta t^2}{2m_p} F_p(t), \quad (8a)$$

$$u_p(t + \Delta t) = u_p(t) + \frac{\Delta t}{2m_p} \left( F_p(t) + F_p(t + \Delta t) \right), \quad (8b)$$

$$\omega_p(t + \Delta t) = \omega_p(t) + \frac{\Delta t}{2I_p} \left( T_p(t) + T_p(t + \Delta t) \right). \quad (8c)$$

The force $F_p(t + \Delta t)$ and torque $T_p(t + \Delta t)$ are computed with the already updated position. Linear acceleration $a_p(t + \Delta t)$ and angular acceleration $\beta_p(t + \Delta t)$ are directly given via $\ddot{F}_p(t + \Delta t)$ and $\ddot{T}_p(t + \Delta t)$ as

$$a_p(t + \Delta t) = \frac{F_p(t + \Delta t)}{m_p}, \quad (9a)$$

$$\beta_p(t + \Delta t) = \frac{T_p(t + \Delta t)}{I_p}. \quad (9b)$$

Rotation is not explicitly accounted for due to the focus on spherical particles. Since inter-particle collisions are not regarded in this work, we do not apply sub-cycling of the particle part and thus make use of the same time step size $\Delta t$ here as in the LBM.36

2.3 Fluid-Particle Coupling

The coupling between the fluid and solid phase is accomplished via the momentum exchange method (MEM-LBM) which has successfully been applied to a variety of particulate flow simulations. The core idea lies in differentiating between solid and fluid cells in the discretized computational domain: A particle is mapped into the fluid simulation by marking the cells it occupies as solid, effectively excluding it from the LBM simulation. This mapping has to be continuously updated for moving particles. This allows for a Lagrangian description of the particle, while the properties of the fluid use an Eulerian model.

In this method, the hydrodynamic interaction force is evaluated as the force acting on the surface of the particle. Within the particle only nodes marked as solid are present. Momentum is transferred solely between the particle boundary and the adjacent fluid, as sketched in the left part of Figure 1. Along the fluid-particle boundary, the particle surface velocity acts as a no-slip boundary condition for the fluid. We here employ the higher-order central linear interpolation (CLI) scheme given by

$$f_q(x, t + \Delta t) = f_q(x, t) + \kappa_0 \Delta t f_q(x - c_q \Delta t, t) - \kappa_0 \Delta t f_q(x, t), \quad (10)$$

with coefficients $\kappa_0 = (1 - 2\delta_q) / (1 + 2\delta_q)$, $\alpha = 4 / (1 + 2\delta_q)$ and where $\tilde{q}$ denotes the opposite direction of $q$. The variable $\delta_q$ describes the ratio between the distance from the fluid cell center to the boundary and the distance from the cell center to the
solid cell center. Therefore, the exact boundary location in direction of the lattice velocity is obtained as $x_b = x + c_q \delta_q$. This introduces subgrid information about the actual boundary location and substantially improves the accuracy to second order, as opposed to the commonly applied simple bounce-back rule that delivers only first order accuracy $^{52,35}$.

The link-based force contribution $F_{q_f-s}$ acting onto a particle at position $x_b$ via a fluid-solid link $q_f-s$ is given as

$$F_{q_f-s}(x_b, t) = \frac{(\Delta x)^3}{\Delta t} \left( \left( c_{q_f-s} - v(x_b, t) \right) \tilde{f}_{q_f-s}(x, t) - \left( c_{q_f-s} - v(x_b) \right) f_{q_f-s}(x, t + \Delta t) \right). \tag{11}$$

Following Ref. $^{55}$ the particle’s surface velocity $v(x_b, t)$ is subtracted from the lattice velocities to ensure Galilean invariance. Summing up over all contributing nodes $q_f-s$, the total hydrodynamic force $F^{hyd}_p$ and torque $T^{hyd}_p$ acting on one submerged particle are obtained:

$$F^{hyd}_p = \sum_{x_b} \sum_{q_f-s} F_{q_f-s}(x_b, t), \quad T^{hyd}_p = \sum_{x_b} \sum_{q_f-s} (x_b - x_p) \times F_{q_f-s}(x_b, t). \tag{12}$$

Updating the explicit particle mapping for a moving particle requires a careful reconstruction of fluid information in cells that gets uncovered in this step. We employ the approach presented in Ref. $^{56}$ which makes use of local velocity gradient information for an improved approximation.

3 | COUPLING TECHNIQUES FOR LIGHT PARTICLES

3.1 | Limitations of Current Approach

To evaluate the approach outlined in Sec. 2 for simulating a light sphere rising in a fluid, we consider the setup shown in Figure 2a with a density ratio $\pi_p = \rho_p / \rho_f < 1$. The setup comprises a single submerged sphere of diameter $d_p$, initially residing at the

- (a) Layout of a simulation for a rising sphere in a periodic simulation domain. The sphere rises in $z$ direction.
- (b) Oscillations in the drag coefficient $c_d$ at $\pi_p = 0.03$, Ga = 170 and $d_p = 40$.  

FIGURE 2 Test case to study the stability of the coupling approach for a sphere rising inside a box.
TABLE 1 Lowest density ratios $\pi_{p,\text{min}}$ at $Ga = 100$ and a certain sphere diameter $d_p$ for which stable results can be obtained with MEM-LBM-coupled LBM and particle phases.

| $d_p/\Delta x$ | 10 | 15 | 20 | 30 | 40 | 50 | 80 |
|----------------|----|----|----|----|----|----|----|
| $\pi_{p,\text{min}}$ | 0.13 | 0.09 | 0.066 | 0.045 | 0.034 | 0.03 | 0.02 |

bottom of the cuboidal domain with dimensions $(6.4, 6.4, 12.8)d_p$. We employ periodic boundary conditions in all directions, and set the initial position of the particle to $(3.2, 3.2, 0.6)d_p$. During the simulation, the particle rises in $z$ direction, as characterized by the Galilei number

$$Ga = \frac{u_g d_p}{v_f}, \quad \text{with} \quad u_g = \sqrt{|\pi_p - 1|g}d_p, \quad (13)$$

where $g$ is the magnitude of the gravitational acceleration and $u_g$ is the characteristic, gravitational velocity. In our simulations, we set $u_g = 0.01$ in lattice units and use $d_p$ to control the overall numerical resolution. Depending on the values for $\pi_p$, $Ga$, and the numerical resolution, the original method can predict the upward motion of the sphere or it may fail by becoming unstable. In the latter case, we observe rapidly growing oscillations of the hydrodynamic force acting on the sphere, as illustrated in Figure 2b for an exemplary case. Here, the hydrodynamic force is expressed in terms of the dimensionless drag coefficient $c_d = 2 F_{hyd}^{p}/\pi_p u_p \pi_p^2$, where $u_z$ is the sphere’s vertical velocity and $r_p = 1/d_p$. With increasing particle density this behavior is delayed to later stages of the simulation until completely disappearing at a certain density threshold. A simulation is considered stable, if no instabilities occurred until the rising sphere has reached its terminal ascension velocity at normalized time $t_n = t/t_g = 10$, with $t_g = d_p/u_g$.

Table 1 lists the minimum density ratio $\pi_{p,\text{min}}$ for which we observe stable results at a certain $d_p$ for $Ga = 100$. Most notably, $\pi_{p,\text{min}}$ behaves close to inversely proportional to the sphere diameter: For instance, at a diameter of 20, 0.066 is the lowest achievable value of $\pi_p$, while at the doubled diameter (40) approximately half the density ratio (0.034) is possible to simulate. The increase in diameter entails a finer resolution of the particle-fluid interface, such that stability issues occur at smaller density ratios. However, every increase in resolution comes with a significant increase in computational costs, such that an alternative approach is required for simulating very light particles efficiently. As such, these observations establish a baseline for possible improvements.

3.2 Analysis of the Instabilities

During each time step of our numerical method, the hydrodynamic interaction forces and torques are first applied to the particle and then a time step for the particle is executed. Thus, these interactions always incorporate a time lag depending on the spatial and temporal resolution. Additionally, also the liquid in the vicinity of a particle must be accelerated together with the particle. This is known as the added mass effect. With an explicit fluid-particle coupling, however, this effect will be accounted for with a time delay. For heavy submerged particles, the added mass effect only plays a minor role and thus does not affect the dynamics. In contrast, for very light particles, the inertial forces originate mainly from the attached fluid mass being accelerated together with the particle. Hence, even though the inherent inaccuracies are minor, they may lead to oscillations whose amplitude grows.

This issue becomes clear by a closer inspection of the equations that describe the temporal evolution of the linear and angular velocity of a single spherical particle submerged in fluid. In general, these equations for geometrically fully resolving simulations are given as

$$\frac{d\mathbf{u}_p}{dt} = \frac{\rho_f}{m_p} \int_S \mathbf{r} \cdot n \, dS + \frac{(\rho_p - \rho_f) V_p}{m_p} g = \frac{1}{\pi_p V_p} \int_S \mathbf{r} \cdot n \, dS + (\pi_p - 1) g = \frac{1}{\pi_p V_p} (F_{hyd}^{p} + F^{\mathbf{g}}) \quad (14)$$

and

$$\frac{d\mathbf{\omega}_p}{dt} = \frac{\rho_f}{I_p} \int_S \mathbf{r} \times (\mathbf{r} \cdot n) \, dS = \frac{1}{2/5\rho_p V_p r_p^2} \int_S \mathbf{r} \times (\mathbf{r} \cdot n) \, dS = \frac{1}{2/5\rho_p V_p r_p^2} T_{hyd}^{hyd} \quad (15)$$

Here, $\mathbf{T}$ is the hydrodynamic stress tensor, $\mathbf{n}$ the normal vector of the particle surface $S$, and $\mathbf{r}$ the vector from the particle center to a point on its surface $S$. For a spherical particle with radius $r_p$, $I_p$ is given as $2/5\rho_p r_p^2$.

For very light particles, i.e. $\pi_p \to 0$, the coupling relations become singular due to a vanishing denominator in Equations 14 and 15. In other cases, a small denominator with $\pi_p \ll 1$ results in a large factor magnifying the fluid contribution.
This amplifies inaccuracies originating from the numerical computation of $F^h_{p}$ and $T^h_{p}$ in explicit fluid-particle coupling approaches\[^{[55]}\].

### 3.3 Virtual Mass Correction for the LBM

This shortcoming for simulations of light particles can be overcome by the virtual mass approach of Schwarz \textit{et al.}\[^{[55]}\]. This approach has originally been developed for a classical Navier-Stokes-based solver in combination with the immersed boundary method (IBM)\[^{[55]}\]. The therein applied IBM originally struggled with density ratios lower than 0.4 due to oscillations in angular and translational velocities leading to a divergence within only few time steps\[^{[55]}\]. This detrimental behavior is therefore similar to the one we observed for the MEM-LBM-coupled simulations.

Here, we aim to employ the same stabilization technique to the LBM with the MEM-based particle coupling, following the arguments provided by Schwarz \textit{et al.}\[^{[55]}\] for the IBM. Alike the IBM, our numerical method accounts for the same Equations (14) and (15). Following Schwarz \textit{et al.}\[^{[55]}\], we introduce the concept of a virtual force

$$F^v_p = m^v_p \frac{du_p}{dt}. \quad (16)$$

It uses the virtual mass $m^v_p = C_v \rho_f V_p$, which introduces the virtual mass coefficient $C_v > 0$. Adding the virtual force $F^v_p$ to both sides of Equation (14) and rearranging yields

$$\frac{du_p}{dr} = \frac{1}{(C_v + \pi_p) V_p} \int_{S} \tau \cdot n \, dS + \frac{\pi_p - 1}{C_v + \pi_p} g + \frac{C_v}{C_v + \pi_p} \frac{du_p}{dr}. \quad (17)$$

A direct comparison with Equation (17) reveals, that this corresponds to a particle with altered mass $m_p + m^v_p$ onto which an additional force $F^v_p$ is acting that exactly compensates the effect of the increased mass. We explicitly note that this virtual force is different from the added mass force, a physically observable effect which is already accounted for in the geometrically fully-resolved simulation model, as we employ it here. The virtual mass coefficient $C_v$ may be determined on an empirical basis. To attain a positive effect, $C_v$ has to be large enough depending on the density ratio. For spherical particles, Schwarz \textit{et al.} propose to use $C_v = 0.5$ referring to the added mass coefficient of submerged spheres\[^{[55]}\]. In our case, values of 0.5 or 1 were found to be suitable, which also satisfy the condition of a lower limit recently reported by Tavanashad \textit{et al.}\[^{[45]}\].

In Equation (17) the derivative of the translational particle velocity appears on either side of the equation. Physically, this is well justified, as the effect induced by the virtual mass should be exactly suppressed by the counteracting force. From an algorithmic perspective, this prevents an explicit temporal integration. As the acceleration in the current time step is to be computed and thus unknown, the acceleration on the right hand side must be approximated to allow explicit integration. Schwarz \textit{et al.} employ second order Lagrange interpolation using the three most recent velocities in order to extrapolate the acceleration\[^{[55]}\]. Here, we alternatively propose to use the particle’s acceleration from the previous time step as computed during the Velocity Verlet procedure (Section 2.2). This essentially simplifies the scheme, reduces memory consumption, and showed the most promising results in our prestudies. Denoting the previous translational acceleration as $a_{p,t-1}$ then leads to

$$\frac{du_p}{dr} \approx \frac{1}{(C_v + \pi_p) V_p} \int_{S} \tau \cdot n \, dS + \frac{\pi_p - 1}{C_v + \pi_p} g + \frac{C_v}{C_v + \pi_p} a_{p,t-1}. \quad (18)$$

Similarly, the equation for angular motion Equation (15) is complemented with a virtual torque

$$T^v_p = \frac{2}{5} C_{v,\alpha} \rho_f V_p^2 \frac{da_{p}}{dr}, \quad (19)$$

where the coefficient $C_{v,\alpha}$ serves the same purpose as $C_v$ for the translational component. Substituting the angular acceleration on the right hand side for an estimate $\beta_{p,t-1}$ and rearranging gives

$$\frac{da_p}{dr} \approx \frac{1}{\frac{2}{5} V_p^2 (C_{v,\alpha} + \pi_p)} \int_{S} r \times (\tau \cdot n) \, dS + \frac{C_{v,\alpha}}{(C_{v,\alpha} + \pi_p)} \beta_{p,t-1}. \quad (20)$$

Consequently, Equations (7a) and (7c) now contain $F_p^v$ and $T_p^v$, such that $F_p = F_p^h + F^v_p$ and $T_p = T_p^h + T^v_p$. The therein applied mass and moment of inertia are now given by $m_p = (\rho_p + C_v \rho_f) V_p$ and $I_p = \frac{2}{5} (\rho_p + C_v \rho_f) V_p^2$, respectively.

Finally, Algorithm 1 outlines the complete simulation algorithm, featuring the steps introduced by the virtual mass correction in green. The update of the flow field via LBM, and the successive computation of the hydrodynamic interactions remains untouched, as well as the computation of the submerged weight force. Then, the virtual force and torque are computed based on
the translational and rotational accelerations of the previous time step. The integrator of the particle is supplied with the virtually increased mass to update the particle’s position and velocities. For the remainder of the paper, we will refer to this approach as \textit{VM-MEM-LBM}, in contrast to the original \textit{MEM-LBM} from Section 2 that does not apply the green parts.

\begin{algorithm}
\caption{Outline of \textit{VM-MEM-LBM} for a single submerged particle.}
\begin{algorithmic}[1]
\item \textbf{for} each simulation step \textbf{do}
\item Perform LBM step.
\item Compute hydrodynamic interactions, and average over two time steps.
\item Set buoyant and gravitational force.
\item Calculate virtual force and torque.
\item Update particle’s translational and angular velocity with virtually increased mass.
\item Update the particle mapping into the fluid domain.
\item \textbf{end for}
\end{algorithmic}
\end{algorithm}

\subsection{Validation}

For validating the translational and angular components of the virtual mass approach, two different scenarios are applied next. For moderate density ratios the unchanged \textit{MEM-LBM}, Section 2, is used as a reference, together with results from Ref. \[45\] where similar validation setups were used.

\subsubsection{Virtual Added Mass Force}

To validate Equation (18), we employ the same setup and parameterization as described in Section 3.1. A first set of simulations are carried out with Galileo number $G_a = 100$ at density ratios $\rho_p \in \{0.1, 1.1\}$ and a resolution of $\Delta_p = 40$, where the \textit{MEM-LBM} serves as a reference. A final test run at $\rho_p = 0.001$, which is well below the minimal density ratio for which we expect stable simulations using \textit{MEM-LBM} and a sphere diameter of 40 cells, employs a Galileo number of 170 and reference data is extracted from Ref. \[45\]. For \textit{VM-MEM-LBM}, we use $C_v = 1$ in all cases.

The normalized ascension velocity of the particle is given as $u_{z,n} = u_z/u_g$. Its mean squared error $\overline{e}_{sq}$ and mean relative error $\overline{e}_{rel}$ with respect to a reference $\hat{u}_{z,n}$ evaluated at $m$ points in time are defined as

\begin{equation}
\overline{e}_{sq} = \frac{1}{m} \sum_{i=1}^{m} (u_{z,n,i} - \hat{u}_{z,n,i})^2,
\end{equation}

\begin{equation}
\overline{e}_{rel} = \frac{1}{\hat{u}_{z,n}} \sum_{i=1}^{m} \frac{u_{z,n,i} - \hat{u}_{z,n,i}}{\hat{u}_{z,n,i}}.
\end{equation}

Additionally, the relative error in the terminal velocity is given as $e_{term,rel} = (u_{z,n,term} - \hat{u}_{z,n,term}) / \hat{u}_{z,n,term}$.

In Figure 3(a), the particle velocities of the simulations employing the \textit{VM-MEM-LBM} are compared with their reference. Overall, all density ratios show very good agreement during the whole simulation. Yet, $\rho_p = 0.001$ deviates slightly from the reference after $t_n \approx 2$. The magnified view of the terminal velocities in Figure 3(b) shows light particles exhibiting an oscillating behavior with small amplitude of less than $0.1\%$ of $u_{z,n}$. For heavier particles, these oscillations cannot be observed.

Visible in Table 2, across all density ratios the \textit{VM-MEM-LBM} performs very well when compared with reference data. The mean relative errors $\overline{e}_{rel}$ amount to less than $0.3 \cdot 10^{-3}$ for all cases with a density ratio $\rho_p \geq 0.1$ (Table 2). However, the mean squared error is much larger in the comparison of the simulation at $\rho_p = 0.1$. This results from fluctuations in the velocities, observable in Figure 3. In the terminal velocity, the relative error $e_{term,rel}$ for the three larger density ratios again is almost nonexistent, listed in Table 2. At an increased terminal deviation of $e_{term,rel} = 4.64 \cdot 10^{-3}$, the error of the simulation with density ratio $\rho_p = 0.001$ is still within reasonable bounds.

Schwarz \textit{et al.} initially report a relative error in the particle velocity of approximately 2% for their general scheme\[45\]. After adjusting the forcing point positions of the particle-fluid-coupling in their simulations they achieve a lower error of $2 \cdot 10^{-3}$, similar to our results.
For the Reynolds number in contrast to the, for this case, unstable MEM-LBM its initial position and all degrees of freedom are blocked at first. The fluid is initialized with a Couette profile, which is further exactly. The proof-of-concept simulation at density ratio and its rotational velocity over time is monitored.

Similar to Ref. 45, this test case features a domain of size \((12.8, 6.4, 4.8)_{d_p}\), confined by two walls in \(z\) direction and periodic otherwise. A sphere of 40 cells in diameter is positioned in the domain center \((6.4, 3.2, 2.4)_{d_p}\). Here, the sphere is kept fixed at its initial position and all degrees of freedom are blocked at first. The fluid is initialized with a Couette profile, which is further driven by the upper moving wall at a constant velocity \(u_w = 0.1\) in \(x\) direction during the simulation. This induces an angular momentum onto the particle, as sketched in Figure 4a. After the flow field has fully developed, rotation of the particle is allowed and its rotational velocity over time is monitored.

The setup is defined by the density ratio \(\pi_p\) and the particle Reynolds number \(Re_p = \frac{u_{\text{z,term}} d_p}{v}\), where \(u_p\) is the undisturbed fluid velocity at the sphere’s position. Since the sphere resides in the center of the domain, the fluid velocity evaluates to \(u_p = \frac{1}{2} u_w\). The Reynolds number \(Re_p = 110\) is chosen to approximately match the situation in the force validation study in Section 3.4.1. For \(\pi_p \in \{0.1, 1.1\}\), we again compare the results to MEM-LBM. Additionally, \(\pi_p = 0.001\) is tested to check stability of VM-MEM-LBM in contrast to the, for this case, unstable MEM-LBM. We define \(t_c = d_p / u_p\) and \(\omega_c = u_p / d_p\) to normalize the time scale and the angular velocity, resulting in \(t_n = t / t_c\) and \(\omega_n = \omega_c / \omega_c\), respectively.

As displayed in Figure 4b simulations that employ the virtual mass correction agree very well to the reference data. The mean relative errors are below \(0.5 \cdot 10^{-3}\) for both cases, see Table 3. We point out that the terminal angular velocities match almost exactly. The proof-of-concept simulation at density ratio 0.001 also appears to have performed well, with a plausible trend in angular velocity and, as expected, a stronger angular acceleration than the heavier spheres.
FIGURE 4 Test case (4a) and error (4b) to validate the VM-MEM-LBM with respect to rotation. While the sphere’s position is fixed throughout the simulation, the upper wall moving with velocity \( u_w \) drives the Couette-initialized fluid, rotating the sphere after free rotation is unblocked.

TABLE 3 Errors in the normalized angular velocity \( \omega_n \) for VM-MEM-LBM compared to simulations using MEM-LBM.

| \( \pi_p \) | 0.1 | 1.1 |
|-----------|-----|-----|
| \( \epsilon_{\text{rel}} \) | 0.46 \( \cdot 10^{-3} \) | 0.15 \( \cdot 10^{-3} \) |
| \( \epsilon_{\text{term,rel}} \) | 0.01 \( \cdot 10^{-3} \) | 0.0 \( \cdot 10^{-3} \) |

3.5 Discussion

We have demonstrated that the virtual mass corrections can be successfully adapted to the momentum exchange method. Thus, the originally observed oscillations in the motion of very light particles are effectively reduced and stable simulations are obtained. As the VM-MEM-LBM relies on an approximation of the particle’s acceleration, the introduction of a certain error in comparison to MEM-LBM is unavoidable, as also observed in Ref. 45. The validation scenarios reveal that this error is very small: In the rising particle setup of Section 3.4.1 the error stays below 0.5\%, for the cases with \( \pi_p \geq 0.1 \) well below that. Evaluating the accuracy of angular motion in Section 3.4.2, the error thresholds for density ratios \( \pi_p \in \{0.1, 1.1\} \) are similarly low at 0.05\%, at most. Nevertheless, even though the virtual mass was introduced as a solely numerically stabilizing technique for explicit fluid-particle coupling schemes, the VM-MEM-LBM might alter the physical results of the simulation. In phases with high acceleration changes, it artificially increases inertia by relying on the past acceleration value. Thus, for those phases, where the virtual force approximation might affect the accuracy negatively, choosing a rather low value of \( C_v \) is advisable. In all our cases, values of 0.5 or 1 were found to be sufficient. These arguments will be revisited in Section 5 where the VM-MEM-LBM again serves to simulate a sphere at \( \pi_p = 0.001 \) and results are compared to literature.

In a recent work, Tavanashad et al. 58 discussed the constant \( C_v \) more extensively and established a lower positive limit for \( C_v \), depending on the density ratio and the added mass coefficient. Our choice of \( C_v \) is in line with this limit.

4 ADAPTIVE GRID REFINEMENT

Accurate numerical studies of particle rising in a fluid, as they will be carried out in Section 5, require large computational domains to reduce the influence of the boundary conditions on the trajectories. On the other hand, ensuring an adequate representation of boundary layers along the particle’s surface and of the vortex structures necessitates a fine numerical resolution in those regions. Using a uniform grid for such simulations would result in enormous computational costs and limit the parameter space that can be explored substantially. To alleviate this problem, we apply adaptive grid refinement in this work which
FIGURE 5 Refinement depending on the presence of a particle. Blocks are outlined black, containing 4x4 cells (outlined blue). (1) In the beginning, the block hosting the particle and its direct neighbors are on the finest level. (2) As soon as the particle enters the next block in vertical direction, the upper left non-refined block notices its presence in one of its lower neighbors and refines. (3) The particle now is fully contained within the upper quarter of the domain, such that the formerly four fine blocks at the bottom all are available to coarsen to one block. The frequency of the refinement evaluations has to be high enough to catch those particle movements, such that it always resides on the finest grid.

significantly reduces the required computational resources. In this section, we briefly outline and validate the grid refinement technique. The method makes use of the domain partitioning functionalities provided by the WALBERLA framework.

4.1 Block-structured Grid Refinement with LBM

Using a block-structured domain partitioning, the computational domain is split into so-called blocks, each containing a lattice of uniformly sized cells. Grid refinement is then carried out by uniformly dividing a block into eight smaller blocks, if needed. A block on the coarsest refinement level then has level \( l = 0 \), while blocks on the finest level have level \( l = l_{\text{max}} \). As each block features the same number of cells, the grid spacing \( \Delta x_l \) of a block gets smaller with increasing level according to \( \Delta x_{l+1} = \frac{1}{2} \Delta x_l \).

Overall, a 2:1 balance between the blocks is maintained, meaning that the refinement level of neighboring blocks must at most differ by one.

A lattice Boltzmann method, capable of dealing with such non-uniform grids, was proposed by Rhode et al. and is applied here. Details about its efficient implementation can be found in Refs. 59,61.

4.2 Refinement Criteria

The refinement structure is defined by the individual target level of each block. Criteria determining the target level are presented below. They are checked regularly throughout the simulation and their result is combined to satisfy all consistency requirements. Subsequently, if some blocks are found to be on an unsuitable level of refinement, the grid is adapted by either coarsening or refining the blocks, obeying the 2:1 restriction.

4.2.1 Particle-based Refinement Criteria

During the simulation, we ensure that blocks that are in the vicinity of particles are always on the finest grid. This is motivated by both algorithmic and physical reasons. From an algorithmic perspective, we avoid the software complexity of maintaining a consistent particle mapping across different refinement levels. At the same time, this refinement rule ensures that the finest resolution is used to resolve the boundary layer around the particle. In these regions high velocity gradients occur and are thus resolved with maximal resolution.

Alternatively, in a block where no particle is nearby, the refinement level would be allowed to become coarser. Here other refinement criteria apply combined with the 2:1 balance between neighboring blocks. A typical scenario is illustrated in Figure 5.

4.2.2 Flow Structure-based Refinement Criteria

Secondly, special algorithmic sensors are applied to the fluid to compute criteria for the refinement of a block. In our case, \( \phi_s \), the scaled curl of the velocity field, is evaluated to detect shear layers and to control the resolution of high velocity gradients:

\[
\phi_s = |\nabla \times \mathbf{u}| s^{(r+1)/r}.
\]
Here, \( \mathbf{u}_f \) denotes the cell local fluid velocity, \( s \) a characteristic length scale for a cell and \( r \) a weighting coefficient. Multiplying by the weighted length scale \( s^{(r+1)/r} \) facilitates the detection of weaker features in a coarser grid area, allowing weaker features to be refined when the stronger ones have been resolved\(^{65} \). The length scale \( s \) can be chosen as \( \sqrt[3]{V_{\text{cell}}} \) with \( V_{\text{cell}} \) as the volume of a cell or, for cubic cells, simply \( \Delta x \). The constant \( r \) is commonly assigned a value of \( 2^{62,63,64} \). A user-defined threshold \( \sigma \) enables the adaptive manner of the fluid phase. Refinement is triggered when \( \phi > \sigma \), while coarsening when \( \phi < \sigma \). To avoid repetitive refinement and coarsening, the value of \( \sigma \) should be lower than \( 1/2^{(r+1)/r} \), i.e. \( \sigma \lesssim 0.35 \) for \( r = 2^{64} \).

### 4.3 Validation

To evaluate the accuracy and performance, we compare adaptive grid refinement against a simulation using a uniform grid. The parameters are chosen to reflect a typical setup as used in the next section. In particular, we use the Galileo number \( G_a = 300 \) and a density ratio of \( 0.5 \) for a sphere of diameter \( d_p = 100 \). These properties do not require the application of VM-MEM-LBM to stably couple solid and fluid phases, such that the MEM-LBM is employed. The domain is fully periodic and of size \((7.68, 7.68, 53.76) d_p\). The sphere is positioned initially at \((3.84, 3.84, 0.6) d_p\). Starting from this point, the sphere rises up to and reaches \( z_n = z/d_p = 50 \) at time \( t_n = 36 \). In that time span we can observe the beginning of a zig-zagging motion as depicted in Figure 7. Based on this scenario, we validate the sphere’s trajectory in an adaptively refining grid against the one in a fully resolved reference simulation.

**FIGURE 6** Domain partitioning at \( t_n \approx 12.5 \) in the adaptive and uniform case. The black lines depict the outline of the blocks. Only the lower region of the simulation domain is shown, where the primary movement direction (\( z \)) of the sphere is from left to right. The vortices around the particle are visualized using the Q criterion\(^{66} \).

In the adaptively refined scenario, we set the refinement threshold \( \sigma \) to 0.001 and the coarsening factor \( c \) to 0.2. According to those values, a block is assigned one of 6 possible levels of refinement. A visual comparison of the resulting domain partitioning for a small part of the domain is provided in Figure 6a, which shows the outline of the blocks, each containing \( 24^3 \) cells. The flow field around the rising sphere is visualized by the Q criterion\(^{66} \) for a time step right before the zig-zagging motion begins.

As the results show in Figure 7, the adaptively refined simulation behaves in the same manner as the one using a uniform grid after the initial trigger of the horizontal motion appears at a slight delay. The particle trajectory resides in a vertical plane, which is rotated by 45° in the horizontal plane. Figure 7a shows the normalized vertical over the horizontal sphere displacement.

By defining a time \( t_o \) at which the horizontal sphere velocity deviates from 0 and thus marks the beginning of the path-instability, we obtain a delay of \( \Delta t_n = t_o^{\text{uniform}} - t_o^{\text{refined}} \approx 0.75 \). This observed delay is attributed to the unpredictable and to a certain degree random appearance of the path-instability. By accounting for this delay while plotting the velocity in Figure 7c the two lines essentially collapse into a single one. A mean relative error between the aligned velocities of 1.1% further underlines the agreement between both simulations and shows that the adaptive resolution introduces no substantial error in predicting the zig-zagging trajectory of the particle.

Regarding the computational resources of both simulations, the respective setup is described in Tab. 4 and was run on the SuperMUC-NG supercomputer at LRZ in Garching. Besides the reduction of the number of cells, the LBM for non-uniform grids carries out less time steps on coarser grids\(^{62} \), which further increases the efficiency of the grid refinement approach. We find that the adaptively refined grid scenario reduced the required total core hours by a factor of 71. In our case, we thus could obtain the essentially same results in less time and using significantly less processes.
As such, we have demonstrated that the here proposed grid refinement approach is capable of drastically reducing the computational costs of such a simulation while maintaining the accuracy of the uniform grid. In combination with the virtual mass correction, this enables efficient simulations of rising particles with very small density ratios.

5 | NUMERICAL STUDY OF RISING PARTICLES

The trajectories of light ascending particles have attracted growing interest since they may exhibit different regimes depending on certain parameters \[ \pi_p \] \[ \text{ and } \text{Ga} \]. With increasing computational power, also numerical simulations became possible. In their work from 2004, Jenny, Dušek & Bouchet showed that the type of trajectory is mainly determined by two parameters, the density ratio \( \pi_p \) and the Galilei number \( \text{Ga} \), which describes the ratio of buoyant and viscous effects. They used numerical simulation to examine the particle paths that are encountered when varying \( \pi_p \in [0, 10] \) and \( \text{Ga} \in [150, 350] \). In their work, they solve the Navier-Stokes equation based on a spectral-element spatial discretization in a cylindrical domain moving with the sphere. In particular, Jenny et al. isolated several regions in the parameter space, where rising spheres would show complex movements. The possible regimes range from steady vertical to three-dimensional chaotic, with an oblique and oblique zig-zagging regime in between.

Horowitz & Williamson performed a comprehensive experimental study across a wide range of sphere densities and Reynolds numbers. Most notably, they identified a “critical mass” ratio, which marked the transition between a steady rise (for a sphere with a density ratio bigger than the critical value) and zig-zagging for a certain Reynolds number beyond the one corresponding to the loss of axisymmetry in the wake. The critical mass ratio amounted to 0.36 ± 0.03 for \( \text{Re} \in [260, 1550] \) and to 0.61 for Reynolds numbers higher than 1550.

More recently, Auguste & Magnaudet carried out an extensive set of simulations using a spectral element method on a moving grid leading to results illustrated here in Figure 8. Plotting the density ratio against the Galilei number, various patterns of motion emerge with increasing Ga and varying \( \pi_p \). Initially they encounter a steady vertical (SV) regime. With further increasing Galilei numbers, steady oblique (SO) and periodic oblique (PO) motion follow. Planar zig-zagging (ZZ) arises next, where
FIGURE 8 Regimes of particle motion characterized by density ratio $\pi_p$ and Galilei number $Ga$ according to Ref. [20]. Overlaid points correspond to our simulations. Numbered triangles mark simulations at least partly differing from Auguste & Magnaudet’s results, circles largely confirm those.

during each change of direction and between two crests vortices are shed. Depending on the density ratio, this regime reportedly persists up to $Ga \approx 250$ for $\pi_p \gtrsim 0.6$ and only up to $Ga \approx 220$ for $0.15 \lesssim \pi_p \lesssim 0.6$. Small amplitude zig-zags for spheres with density ratio of $\gtrsim 0.6$ in a three dimensional regime termed ZZ$_2$ follow next; at lower density ratios an intermittent regime (IT) up to $Ga \approx 250$ occurs first. In a small stride of the map, very light spheres perform oblique zig-zagging (ZO). After a threshold value of $Ga \approx 250$ to 300, three dimensional chaotic (3DC) paths are assumed by submerged spheres of all density ratios. Beyond $Ga \approx 400$ however, some regularity is regained in the spiraling motion (SP) for very light spheres.

Except for some differences at $Ga = 200$ to 250, these findings agree largely with the ones from Zhou & Dušek [19], who used a similar numerical method. On the other hand, these numerical results show deviations from the experimental studies of Horowitz & Williamson, who e.g. do not record sphere trajectories pertaining to the 3DC regime.

In the present work, we study 16 combinations of $Ga$ and $\pi_p$ that we simulate with the new method as proposed in this article, if required. This allows us to further validate our method on the one hand, and to investigate the parameter spaces where existing studies report mismatching results. The analyzed parameter combinations are marked in Figure 8.

5.1 Simulation Setup

All simulations are performed in a cuboidal simulation domain with periodic boundary conditions in all directions. Large enough domains are chosen to avoid that turbulent structures spread so far that they would influence the particle wake or the trajectory by re-entering on the opposite side of the domain. Depending on the combination of $Ga$ and $\pi_p$, the sphere is resolved using a varying number of cells per diameter, expressed by $d_p/\Delta x$, to assure a fine enough resolution of the boundary layer along the sphere surface and the wake. We adjust the parameter $\Lambda_b$ of the MRT collision operator as introduced in Section 5.1 to $\Lambda_b = 1$, which recovers the TRT collision operator.

In all cases, adaptive grid refinement, as described in Section 4, is applied to reduce the computational cost. Depending on the domain size, 8 or 9 levels of refinement are applied. The necessity for an adaption of the grid is evaluated every 4 to 8 time steps on the coarsest grid level. The flow-based refinement criterion from Section 4.2.2 uses $\sigma_c = 0.001$ and $c = 0.2$. Similar to the simulations described in Section 3, the gravitational velocity $u_g = 0.01$ in lattice units is used which then determines the gravitational acceleration and the kinematic viscosity for the simulation. A summary of the domain size, $d_p$ and refinement levels for each of the setups is presented in Table 5. The virtual mass approach from Section 3 in the fluid-solid coupling is only employed when it is required for stable simulations. In the present cases, this is in settings where the particle density $\pi_p = 0.001$. Then, the virtual mass coefficients are chosen as $C_v = C_{v,0} = 0.5$. 
TABLE 5 Domain properties and sphere resolution \( d_p/\Delta x \) used for the simulations of this chapter. Refinement check frequency is expressed in terms of time steps on the coarsest grid level.

| Setup | Domain Size | \( d_p/\Delta x \) | Refinement Levels | Refinement Check Freq. |
|-------|-------------|-----------------|------------------|-----------------------|
| I     | (38.4, 38.4, 192) | 80              | 8                | 4                     |
| I'    | (38.4, 38.4, 384) | 80              | 8                | 4                     |
| II    | (30.72, 30.72, 215.04) | 100             | 8                | 4                     |
| III   | (38.4, 38.4, 307.2) | 160             | 9                | 8                     |

5.2 Simulation Results

The 16 simulations range over a Galilei numbers from 150 to 500 at particle densities of 0.5, 0.1, 0.05, 0.01 and 0.001. The results for the key indicators are concisely summarized in Table 5. The parameters are selected such that the range of regimes from the existing literature is covered. In particular, we follow Auguste & Magnaudet’s extensive study and perform a subset of their simulations, plus two additional cases (Case 13 and 16 in Table 6).

Cases 1, 3 and 4 match with the descriptions by Auguste & Magnaudet well, pertaining to the simpler patterns of steady vertical or oblique movement. However, a disagreement is found for Case 2 where the Galilei number is specifically chosen to be located in the transition regime between SV and SO. Auguste & Magnaudet identify the SO regime here, while in our simulation the sphere appears to move SV with visible transitions to an oblique motion.

In the next four cases, 5 to 8, we fix the Galilei number at 200, merely varying the density ratio. Here we observe three different regimes: ZZ, 3DC, and PO. While we find agreement with Auguste & Magnaudet for Cases 5 and 8, simulations 6 and 7 do not produce the PO trajectories as reported by Auguste & Magnaudet. Instead, we observe a chaotic motion of the sphere, only in Case 6 initially resembling a PO path. However, Zhou & Dušek also categorize those into the 3DC regime.

Further increasing the Galilei number and setting the density ratio to 0.5 in Cases 9 to 11 shows agreement with Auguste & Magnaudet. In addition to the already established ZZ regime in Cases 9 and 10, a second zig-zagging motion, ZZ\(_2\), is identified in Case 11. This is characterized by a higher frequency and a smaller amplitude.

The final five scenarios feature the largest Galilei numbers. They all exhibit a spiraling motion, except Case 14. There, the trajectory loses all regularity resulting in three-dimensional chaotic motion. These findings are again in agreement with Auguste & Magnaudet. Additionally, Zhou & Dušek confirms our results in Cases 13 and 16, since our results for very light spheres (density ratio of 0.001) match their results for massless spheres.

All in all, we identify similar issues as both previous numerical studies in replicating the experiments of Horowitz & Williamson. A “critical mass ratio” and zig-zagging motion instead of three dimensional chaotic motion at increasing Reynolds numbers could not be found.

5.3 Detailed Analysis of Results

In the following subsections, we describe our simulation results in more detail, following the analysis provided by Zhou & Dušek and Auguste & Magnaudet. This enables an in-depth comparison with these studies, based on various quantities of interest that are also provided in Table 6.

In the following, all reported particle displacements are normalized in terms of the sphere diameter \( d_p \). As such, normalized coordinate axes corresponding to the particle’s trajectory are denoted as \( x_n, y_n \) and \( z_n \). To quantify periodic paths, a dominant frequency \( f \) can be defined and expressed as the dimensionless Strouhal number \( St = f d_p/u_z,t \), see Ref. [20]. Here, the quasi-steady vertical velocity \( u_z,t \) during the rise of the particle serves as reference velocity, normalized beforehand using the gravitational velocity \( u_g \). The frequency of sphere oscillations is computed by a Fast Fourier transformation of the horizontal component of the velocity and extracting the frequency with the highest amplitude. For comparison with Zhou & Dušek, we compute the normalized frequency as \( f_n = f t_g \). Further, the lateral displacement \( d_{cr} \) and height \( h_{cr} \) are determined from one typical “zig-zag” or one circle of the spiral. Inclination angles with respect to the vertical axis are computed by fitting a straight line by means of linear regression, starting at the beginning of the oblique displacement.
TABLE 6 Results for simulations of a rising sphere at various combinations of Galilei number $Ga$ and particle density ratio $\pi_p$. For comparison, regimes as found by Auguste & Magnaudet (AM) and Zhou & Dušek (ZD) are provided next to ours. Abbreviations are explained in Figure 8. Columns labeled $u_{z,t}$, $t_{n,t}$ and $z_{n,t}$ list the normalized terminal values of the respective quantity. $d_{cr}$ and $h_{cr}$ describe the lateral distance and height from one crest to the following crest after completing one iteration of either a spiraling or a zig-zagging path. Regimes from literature are mostly backed by simulations in the respective case; instances, where only a visual classification by diagram is available, are marked with (*).

| Case | Setup | Ga  | $\pi_p$ | Regime AM | ZD | Re  | Incl. [°] | St  | $d_{cr}$ | $h_{cr}$ | $u_{z,t}$ | $z_{n,t}$ | $t_{n,t}$ |
|------|-------|-----|---------|-----------|----|-----|-----------|-----|----------|----------|-----------|-----------|----------|
| 1    | I     | 150 | 0.5     | SV        | SV | 196.2| 1.309     | 191.8| 147.9    |           |           |           |           |
| 2    | I     | 162.5| 0.5    | SV        | SO  | 218.2| 1.343     | 191.8| 143.1    |           |           |           |           |
| 3    | I     | 172 | 0.5     | PO        | SO  | 232.0| 0.043     | 191.8| 145.4    |           |           |           |           |
| 4    | I     | 175 | 0.5     | PO        | ZZ,PO| 237.0| 0.042     | 1.348| 262.6    |           |           |           |           |
| 5    | II    | 200 | 0.5     | ZZ        | ZZ  | 277.8| 0.018     | 1.46 | 214.8    | 155.2    |           |           |           |
| 6    | II    | 200 | 0.1     | 3DC      | PO  | 277.5| 1.356     | 214.8| 155.1    |           |           |           |           |
| 7    | II    | 200 | 0.05    | PO, 3DC  | PO  | 277.9| 2.90      | 214.8| 155.3    |           |           |           |           |
| 8    | II    | 200 | 0.001   | PO        | 3DC  | 276.9| 3.07      | 145.0| 155.6    |           |           |           |           |
| 9    | II    | 212.5| 0.5    | ZZ        | ZZ,ZZ| 299.1| 0.028     | 1.14 | 241.5    | 172.6    |           |           |           |
| 10   | II    | 237.5| 0.5   | IT, ZZ    | ZZ,ZZ| 344.5| 1.34      | 0.098| 1.449    | 254.9    | 177.9    |           |           |
| 11   | II    | 300 | 0.5     | ZZ,ZZ    | 3DC  | 447.9| 0.099     | 0.28 | 1.495    | 238.3    | 162.1    |           |           |
| 12   | III   | 400 | 0.01    | SP        | SP  | 591.0| 0.070     | 14.20| 171.9    | 117.3    |           |           |           |
| 13   | III   | 400 | 0.001   | SP        | SP* | 586.6| 0.070     | 14.06| 294.9    | 201.0    |           |           |           |
| 14   | III   | 500 | 0.5     | 3DC      | 3DC  | 815.2| 1.600     | 167.2| 105.0    |           |           |           |           |
| 15   | III   | 500 | 0.05    | SP        | 3DC  | 757.3| 0.067     | 1.08 | 266.3    | 177.6    |           |           |           |
| 16   | III   | 500 | 0.001   | SP        | SP* | 729.3| 0.20      | 1.09 | 264.8    | 181.0    |           |           |           |

5.3.1 Galilei Numbers $Ga \leq 175$: Steady Vertical and Oblique

Cases 1 to 4 of Table 6 feature Setup I, covering Galilei numbers from 150 to 175 at a density ratio of 0.5. We observe steady vertical and oblique movement for these simulations.

At Galilei number 150 (Case 1), the sphere rises in a steady vertical line, with only very minor lateral displacement. This is in line with findings of both Auguste & Magnaudet and Zhou & Dušek.

Case 2 at $Ga = 162.5$ still shows movement corresponding to the SV regime. Yet for Auguste & Magnaudet, this case marked the transition to a second regime with steady oblique movement. A closer inspection of our obtained trajectory hints at a transition to obliqueness (Figure 9b), which supposedly is triggered at a slightly higher Galilei number. Unlike Case 1, the path is less oscillating around a vertical axis, but shows especially for the $y$ direction obliqueness with lateral displacement in the order of one tenth of the sphere diameter.

Oblique paths are first observed for Case 3 at $Ga = 172$. This is the first occurrence of a PO path, and corresponds well with Auguste & Magnaudet. Further considering the inclination angle between the trajectory and the vertical axis, Auguste & Magnaudet reported an average value of approximately $4.5°$, in comparison to $4.6°$ in our case. The comparison Strouhal number $St = 0.05$ is close to the one at hand (0.043). Figure 9c depicts the wake behind the rising particle: The sphere is constantly enclosed by a flow that builds up and sheds two axisymmetric fluid tubes in regular intervals.

The last case, 4, uses the enlarged Setup I to capture a longer impression of the trajectory. The general motion stays the same compared to Case 3, with the inclination slightly changing to $4.74°$. Auguste & Magnaudet there noticed zig-zagging at first, which, however, ends after some iterations and changes to an oblique movement, like observed here right from the beginning.

5.3.2 Galilei Numbers $200 \leq Ga \leq 300$: (Oblique) Zig-Zagging and Three Dimensionally Chaotic

A series of six simulations (Cases 5 to 11) using Setup II features Galilei numbers between 200 and 300 at various density ratios, as low as $\pi_p = 0.001$. Following these parametric alterations, vertical and oblique zig-zagging and three dimensionally chaotic regimes emerge.

Various trajectory types are observed at a Galilei number of 200 and three different density ratios. Planar and regular zig-zagging occurs for Case 5 at $\pi_p = 0.5$, as can be seen in Figures 10a and 11a, where the lateral displacement during each ZZ
iterative measures about 1.5d_p. The Strouhal number is St = 0.025. Auguste & Magnaudet did not state detailed numbers for this set of parameters, yet depicted the corresponding path, which matches with ours in Figure 10a (blue). Zhou & Dušek more extensively reported on this case, providing a frequency spectrum of the horizontal velocity. They noticed a main peak at f_n = 0.035, which coincides with ours very well (0.035). The same can be stated about a second, smaller peak at f_n = 0.10. Furthermore, the descriptions of the particle motion correspond well.

Case 6 lowers the density ratio to 0.1, yielding an irregular zig-zagging pattern with some obliqueness up to zn ≈ 100 (Figure 10a). Also, three-dimensional motion up to a certain degree is observed. As such, no Strouhal number can be determined. This differs from Auguste & Magnaudet, who report periodic oblique paths here. Only the initial phase up to zn ≈ 70 agrees qualitatively with their simulations.

Similar observations are made for Case 7 at \( \pi_p = 0.05 \) in Figure 10b, which starts with a regular PO movement, continues obliquely with reduced periodicity and ends chaotic after rising up to zn ≈ 160. Up until that point, the average inclination of 2.9° falls within the range of < 3° reported by Auguste & Magnaudet. In Case 8, a density ratio of \( \pi_p = 0.001 \) is simulated by utilizing the VM-MEM-LBM. Initially, the path resembles the one of the previous Case 7, but stays approximately planar. Additionally, its average inclination of 3° does not change much during its periodic zig-zags, such that this case can be assigned to the PO regime. As such, a Strouhal number of 0.045 for the dominant frequency \( f_n = 0.063 \) can be determined. Worth mentioning is the emergence of a second not as pronounced frequency at \( f_n = 0.111 \) with St = 0.079. While Zhou & Dušek did not provide detailed results on the last three cases, their provided classification suggests chaotic movement for Ga = 200 and \( \pi_p \leq 0.2 \).

Case 9 is displayed in Figure 12 where the sphere’s motion at Galilei number of 212.5 and density ratio of 0.5 behaves comparable to Case 5. It corresponds to the ZZ regime, slightly tilting its original zig-zagging plane beyond \( z_n \approx 180 \). The projected horizontal displacement of the zig-zagging of approximately 1.5d_p is also similar. Auguste & Magnaudet identified a Strouhal number ranging from 0.016 to 0.036, confirming ours at St ≈ 0.028.

Figure 11B illustrates the trajectory of a particle at Ga = 237.5 and \( \pi_p = 0.5 \), corresponding to Case 10. The path starts as ZZ until \( z_n \) reaches 100 with a Strouhal number of St ≈ 0.03, having a large amplitude. Afterwards it enters a slightly inclined plane (1.37°) with the periodic frequency increasing strongly, leading to St ≈ 0.10. This is different from the findings of Auguste & Magnaudet, displaying a movement more prevalent for them at higher Galilei numbers between 250 and 300. At this point, the sphere possibly already enters their ZZ_2 regime, causing a much larger Strouhal number. When considering the simulation at

**FIGURE 9** Cases 1 to 4: Plots (a, b) show trajectories at \( \pi_p = 0.5 \): Ga = 150 (magenta), 162.5 (green), 172 (orange) and 175 (red). Solid lines correspond to movement in x direction, dashed in y direction. In (c) the wake structure of Case 3 is visualized using the Q criterion at a threshold of 10^{-10} and colored by normalized vorticity (between −3.3, blue, 0 in green and 3.8, red).
FIGURE 10 Cases 5 to 11: Trajectories for the range of Galilei numbers between 200 and 300. Combinations of Galilei number and density ratio depicted as follows. Ga = 200: $\pi_p = 0.5$ (blue), $\pi_p = 0.1$ (green), $\pi_p = 0.05$ (orange), $\pi_p = 0.001$ (purple); Ga = 212.5: $\pi_p = 0.5$ (red); Ga = 237.5: $\pi_p = 0.5$ (cyan); Ga = 300: $\pi_p = 0.5$ (brown).

FIGURE 11 Cases 5, 10 and 11: Various cases of zig-zagging in their vertical and horizontal (projected to xy plane) movement.

Ga = 240 and $\pi_p = 0.5$ by Zhou & Dušek as reference, their results match with ours with the exception of initial large-amplitude zigzagging, as described. 

ZZ$_2$ is also the regime in which Case 11 with a Galilei number of 300 and density ratio of 0.5 is placed. Its spatial progression is depicted in Figure 11c. Different from Auguste & Magnaudet’s simulation, we observe an initial lateral swing of magnitude 2$d_p$, before a more regular oscillatory path is taken. Furthermore, their Strouhal number approximately coincides with ours, at
FIGURE 12 Case 9: Vortices behind a sphere of density ratio 0.5 at $Ga = 212.5$. Depicted are the states before and during movement through a crest of zig-zagging. A $Q$ criterion threshold of $10^{-10}$ is employed and coloring is done by normalized vorticity, which ranges between -4 (blue) and 4 (red), green corresponding to 0.

(a) Case 12: $Ga = 400, \pi_p = 0.01$: SP.  
(b) Case 14: $Ga = 500, \pi_p = 0.5$: 3DC.  
(c) Case 16: $Ga = 500, \pi_p = 0.001$: SP.

FIGURE 13 Cases 12, 14 and 16: At $Ga = 400$ and above, two regimes are found: Three dimensional chaos (3DC) and spiraling (SP).

$St = 0.10$. The distance from crest-to-crest is $0.3d_p$, as in Auguste & Magnaudet. More so, their observation of a rotating zig-zag plane can be confirmed (see $xy$ plot in Figure 11c). The findings of Zhou & Dušek also agree with ours.

5.3.3 Galilei Numbers $Ga \geq 400$: Spiralling and Three Dimensionally Chaotic

The last simulations cover Galilei numbers of 400 and 500, corresponding to Cases 12 to 16. Depending on the density ratio, we encounter either chaotic movement or a highly regular spiraling regime.
This new regime is found for Case 12 at Ga = 400 and \( \pi_p = 0.01 \). The spiraling begins after an initial phase, which transforms from planar zig-zagging up until \( t_n = 40 \) to a three dimensional movement. After \( t_n = 80 \) the projection of the trajectory onto the xy plane resembles an ellipsis closely approaching the shape of a circle with a diameter of \( 1d_p \). The vertical stride between the spiraling iterations is approximately \( 14.2d_p \), resulting in \( St \approx 0.07 \). While not matching perfectly with Auguste & Magnaudet, these numbers come close to their spiral diameter \( 1.3d_p \) and Strouhal number of approximately \( 0.07 (13.5d_p \) stride).

Case 13 decreases the particle density ratio further to \( 0.001 \) at \( Ga = 400 \) with the aid of the virtual mass approach. The vertical crest-to-crest distance changes to \( 14.06d_p \), while the Strouhal number stays the same. Equally, the diameter of the spiral varies only to a very minor degree. Zhou & Dušek provided results of an approximately massless sphere at this Galilei number. Its trajectories match ours, however pitch (\( 12.6d_p \) theirs, \( 14.06d_p \) ours) and terminal vertical velocity (\( 1.382 \) theirs, \( 1.466 \) ours) differ to a certain degree.

Continuing with Case 14, we observe the emergence of a three dimensional chaotic region, simulated here using a Galilei number of 500 and density ratio of 0.5. This path is highly irregular and shows no sign of periodicity (Figure 13b). The occurrence of 3DC trajectories at this parameter combination was also observed by Auguste & Magnaudet and Zhou & Dušek.

Case 15 features a particle of density ratio \( 0.05 \) and Galilei number 500. Again, the particle takes up a SP path, albeit with an increased duration of the initial transition compared to the particle of Cases 12 and 13 at \( Ga = 400 \). Even though at \( \pi_p = 0.001 \), Figure 13c shows approximately the same delay as \( \pi_p = 0.05 \). The vertical stride of the spiral reduces slightly to \( 13.8d_p \) at a horizontal displacement of \( 1d_p \), which is reflected in an increased Strouhal number \( St = 0.067 \). In this instance, no reference data is available for a direct comparison. Zhou & Dušek performed two simulations at the same Galilei number and density ratios of 0.1 and 0; their depicted trajectory of \( \pi_p = 0.1 \) reflected the notion of the present transient from planar zig-zagging to a spiralling path. Their resulting Reynolds number of 750 confirms ours at \( Re \approx 757 \). After entering the quasi-steady state, the particle of Case 15 moves vertically with \( u_{z,n} = 1.512 \), which places close to Zhou & Dušek’s at 1.406 (\( \pi_p = 0 \)) and 1.501 (\( \pi_p = 0.1 \)). Radius and pitch of the trajectory closely approach Zhou & Dušek’s as well.

Case 16 displays a modification of the SP trajectory (Figure 13c), where the particle at \( \pi_p = 0.001 \) and \( Ga = 500 \) takes up a slightly inclined spiraling path (inclination angle \( \approx 0.2^\circ \)). Such behavior is also observed by Auguste & Magnaudet, who found the corresponding motion already at \( \pi_p = 0.01 \). The spiral is described by a diameter of \( 1.09d_p \) and vertical stride of \( 13.22d_p \); the movement along this spiral by \( St = 0.074 \) and \( u_{z,t} = 1.455 \).

6 Conclusion

In this work, we present an improved LBM for simulations of light particles submerged in a fluid, including a comparison with previously established methods. This is based on a set of benchmarks that are chosen to expose specific difficulties and peculiarities arising in systems of submerged particles with density ratios \( \ll 1 \). In order to achieve stable simulations without excessively fine resolution, we adapt and apply the virtual mass approach of Schwarz et al.\( ^{[45]} \) resulting in the improved VM-MEM-LBM. The underlying idea is to artificially increase the mass of the particle to avoid an otherwise vanishing denominator that would amplify inaccuracies of the fluid-particle coupling scheme. This is exactly compensated by an appropriate force and torque, which in practice requires an approximation of the spheres translational and rotational acceleration. This approach is shown to enable density ratios of 0.001 and which would thus permit e.g. the simulation of spherical air bubbles in water. The numerical stabilization scheme is validated both with respect to the accuracy of rotational and translational velocities.

In order to further increase the computational efficiency of the parallel LBM code, we employ adaptive grid refinement. This ensures an adequate and accurate representation of the flow features while permitting large computational domains. Areas in need of refinement are identified by employing sensors evaluating the state of the fluid and the solid phase. The evaluation of the grid adaptation criteria is invoked at regular time intervals. For the case of a rising sphere, the computational cost could be reduced by a factor of 71, when compared to executing same simulation scenario on a uniform fine grid. This is achieved while the accuracy is essentially unaffected.

The efficiency improvement supplied by the adaptive grid refinement algorithm is finally applied in 16 distinct simulation scenarios that study the trajectories of a single rising sphere. In the cases of smallest density ratio of 0.001, the virtual mass approach proved to be essential to reach a stable time stepping. A multitude of different trajectory types is observed and the results are compared to data from the literature. This includes trajectory classes such as vertical to oblique, zig-zagging, spiraling, three dimensional chaos, and intermittent motion. In many cases good agreement to experimental and numerical studies could be found, for the broad classification via the regimes but also for specific parameters like terminal rising velocities and oscillation.
FIGURE 14 Case 15: Vortices behind a sphere of density ratio 0.05 at Ga = 500. In frames 4 and 5 the three vortex threads delivering a constant torque to the ascending sphere are well visible. A Q criterion threshold of $10^{-10}$ is employed and coloring is done by normalized vorticity, which ranges between -10 (blue) and 10 (red). Lighter colors correspond to stronger magnitude.

frequencies. This served as a further validation of the here presented approach and showcased its applicability for predictions of complex particle dynamics. In some cases, the existing literature provided contradicting statements regarding the observed regime of motion and we observed supporting arguments for one or the other.

We note that while validated here for single spherical particles, our new method is neither restricted to a single particle nor to spherical shapes. The VM-MEM-LBM is also suitable for a wide range of physical parameters, and it can be employed in domains of arbitrary shape. This is considered a major improvement to the numerical schemes applied previously in the simulation studies of trajectories of rising particles. A massively parallel and efficient implementation is available in the open-source WALBERLA framework\cite{32}, enabling the simulation of ensembles of several submerged particles and to study their collective motion. Such studies will be the topic of future research.

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