



# A comparative study of fluid-particle coupling methods for fully resolved lattice Boltzmann simulations



C. Rettinger<sup>a,\*</sup>, U. Rude<sup>a,b</sup>

<sup>a</sup>Chair for System Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Cauerstraße 11, 91058 Erlangen, Germany

<sup>b</sup>CERFACS, 42 Avenue Gaspard Coriolis, 31057 Toulouse Cedex 1, France

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## ABSTRACT

The direct numerical simulation of particulate systems offers a unique approach to study the dynamics of fluid-solid suspensions by fully resolving the submerged particles and without introducing empirical models. For the lattice Boltzmann method, different variants exist to incorporate the fluid-particle interaction into the simulation. This paper provides a detailed and systematic comparison of two different methods, namely the momentum exchange method and the partially saturated cells method by Noble and Torczynski. We discuss their algorithmic parts in detail, show and propose improvements to the commonly applied algorithms, and eventually identify three suitable subvariants of each method. These subvariants are used in the benchmark scenario of a single heavy sphere settling in ambient fluid to study their respective strengths and weaknesses in accurately reproducing characteristic physical phenomena for particle Reynolds numbers from 185 up to 365. The sphere must be resolved with at least 24 computational cells per diameter to achieve velocity errors below 5%. The momentum exchange method is found to be more accurate in predicting the streamwise velocity component whereas the partially saturated cells method is more accurate in the spanwise components. The study reveals that the resolution should be chosen with respect to the coupling dynamics, and not only based on the flow properties, to avoid large errors in the fluid-particle interaction.

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## 1. Introduction

To study particulate flows, direct numerical simulations (DNS) have become a viable and important tool. Resolving the flow structures and the submerged particles offers the unique possibility to trace the motion of single particles, to evaluate the hydrodynamic forces acting on each individual particle, and to investigate the flow field in detail. As an alternative to conventional computational fluid dynamics (CFD) methods that solve the Navier–Stokes equations, the lattice Boltzmann method (LBM) has been applied successfully for DNS studies of such particulate systems. Examples include coupled simulations of several thousand [1,2] up to millions of spherical particles [3,4] as they typically appear in fluidized beds at a laboratory scale. Also non-spherical objects can be handled by this method which allows to study flows with blood cells [5], the motion of elongated particles [6,7] and ice floes [8]. Extensions exist that incorporate electrostatic forces between the particles [9,10], enable deformable objects [11,12] or model self-propelled swimmers [13].

A crucial component of such simulations is the accurate and efficient description of the interaction between the solid and the fluid phase which requires appropriate coupling methods. Avoiding the costly remeshing due to changes in the geometry and topology that are caused by the moving particles is a key aspect here. Therefore, classical CFD methods often make use of the immersed boundary method to satisfy the no-slip boundary condition on the particle surfaces and to compute the hydrodynamic forces acting on them [14–16]. The standard LBM employs uniform Cartesian meshes with cubic cells and thus it is natural here that coupling methods are utilized which do not alter the mesh. This results in an excellent parallel performance and scalability of the LBM method [17,18] and with suitable data structures also the fluid-solid coupling can be implemented with high parallel efficiency [4,19].

Several different fluid-solid coupling approaches have been proposed for the LBM: the momentum exchange method [20,21], the partially saturated cells method [22,23], and methods that rely on Lagrangian marker points like the immersed boundary method [24–26] or the external boundary force method [11]. Recently, another method referred to as homogenized LBM has been proposed

\* Corresponding author.

E-mail address: [christoph.rettinger@fau.de](mailto:christoph.rettinger@fau.de) (C. Rettinger).

[27]. Beyond this general classification of the methods, a large number of subvariants can be found in literature.

It is apparent that a rigorous systematic comparison of these methods for systems with moving solid particles is needed to assist the choice for a suitable method. Challenges here are to define appropriate benchmark scenarios for which reliable reference data exist and to cover the flow regimes at larger Reynolds numbers as they are most relevant for typical engineering applications. One standard benchmark is to evaluate the drag force acting on an infinite periodic array of spheres in Stokes flow, as e.g. in [28–31]. This benchmark can make use of an analytic solution in the form of a series expansion [32,33] and is thus particularly suitable to validate implementations and investigate certain characteristics of the fluid-solid coupling methods as will be demonstrated later on in this article. However, the significance of this benchmark is limited when the goal is to simulate scenarios with moving particles at larger Reynolds numbers since the motion of the particles will affect the accuracy and stability of the coupling mechanism. A suitable benchmark has to take into account all possible sources of numerical errors that might appear in a coupled simulation. Besides the fluid simulation itself, errors can be introduced by the particle simulation and the coupling from the fluid to the solid phase and vice versa.

Some studies exist that aim at directly comparing different fluid-solid coupling methods for LBM but they are mostly restricted to two-dimensional setups: In [28], the momentum exchange method with an interpolated bounce back scheme and the immersed boundary method are compared with respect to their accuracy and efficiency for a laminar flow over a stationary cylinder [34]. The settling of circular and elliptical particles is simulated in [35] to establish a comparison between three different LBM collision operators in combination with the momentum exchange method. Various coupling methods are compared in [36] for two-dimensional objects with a prescribed motion and with the focus on the accuracy of acoustic properties. In a recent study, sedimentation of a single circular particle is simulated with different coupling methods [37].

The benchmark proposed by Uhlmann and Dušek [38] features a single sphere settling in an ambient fluid in a three-dimensional domain. High accuracy results obtained with spectral elements are available for flow regimes with particle Reynolds numbers ranging from 185 up to 365. This test case can be set up independent of the used CFD method and it is well suited to compare different methods with respect to their ability to reproduce characteristic physical phenomena accurately. Its applicability to LBM has already been demonstrated in a preparatory study by [39]. In particular, it can be used to evaluate which resolution is required to achieve sufficiently accurate results in these flow regimes. In this article, we therefore use this benchmark to establish a systematic comparison between two commonly used coupling approaches with the LBM, namely the momentum exchange method and the partially saturated cells method. For each method, three distinct subvariants are proposed, applied and validated to illustrate their respective features and strengths. For the momentum exchange method, the simple bounce back and two interpolated versions are compared, whereas different solid collision operators are used for the partially saturated cells method. Methods that employ Lagrangian markers are not included in this study as they are typically more suitable for deformable objects in contrast to the rigid particles here. However, future work should also investigate those methods to establish a complete overview over all available coupling methods.

The remainder of this paper is structured as follows: First the numerical methods are introduced in Section 2. This includes a brief summary of the lattice Boltzmann method in Section 2.1 as basis for the momentum exchange method and its variants presented in Section 2.2. The partially saturated cells method with

its variants is introduced in Section 2.3. A short validation study in Section 3 compares the obtained force on a fixed sphere in Stokes flow for the resulting six approaches. Section 4.1 elaborates the setup of the benchmark test case from Uhlmann and Dušek. The six coupling approaches are then evaluated for four different flow regimes in Sections 4.2–4.5. The results are discussed in Section 4.6. Finally, the most important findings are summarized in Section 5.

## 2. Numerical method

### 2.1. Lattice Boltzmann method

For the simulation of hydrodynamics, the lattice Boltzmann approach [40] with the *D3Q19* lattice model [41] is utilized. Having its origin in statistical mechanics, the evolution of particle distribution functions (PDFs) on a Cartesian lattice is computed by solving the lattice Boltzmann equation. Each of these PDFs  $f_q$ , with  $q \in \{0, \dots, 18\}$ , is associated with a lattice velocity  $\mathbf{c}_q$ . The lattice Boltzmann equation is usually split into the collision and the streaming step. In its most general form, the collision step is given by

$$\tilde{f}_q(\mathbf{x}, t) = f_q(\mathbf{x}, t) + C_q(\mathbf{x}, t) + \mathcal{F}_q(\mathbf{x}, t), \quad (1)$$

specified by the collision operator  $C_q$  and the external forcing operator  $\mathcal{F}_q$ . In the succeeding stream step, the post collision values  $\tilde{f}_q$  are distributed to the corresponding neighbor lattice cells via

$$f_q(\mathbf{x} + \mathbf{c}_q \Delta t, t + \Delta t) = \tilde{f}_q(\mathbf{x}, t). \quad (2)$$

The most commonly applied collision model is the BGK model [42] that uses a single relaxation parameter to linearly relax the PDFs towards their equilibrium values  $f_q^{\text{eq}}$ . Those can be computed as

$$f_q^{\text{eq}}(\rho_f, \mathbf{U}) = w_q \left( \rho_f + \rho_0 \left( \frac{\mathbf{c}_q \cdot \mathbf{U}}{c_s^2} + \frac{(\mathbf{c}_q \cdot \mathbf{U})^2}{2c_s^4} - \frac{\mathbf{U} \cdot \mathbf{U}}{2c_s^2} \right) \right) \quad (3)$$

for incompressible flows [43]. The fluid density  $\rho_f = \rho_0 + \delta\rho_f$ , with the mean density  $\rho_0$  and the fluctuation  $\delta\rho_f$ , and the velocity  $\mathbf{U}$  are cell local quantities and calculated via moments of the PDFs:

$$\rho_f(\mathbf{x}, t) = \sum_q f_q(\mathbf{x}, t), \quad \mathbf{U}(\mathbf{x}, t) = \frac{1}{\rho_0} \sum_q f_q(\mathbf{x}, t) \mathbf{c}_q. \quad (4)$$

The lattice weights  $w_q$  are as given e.g. in [41] and  $c_s$  is the lattice speed of sound. The collision operator for the BGK model is then

$$C_q^{\text{BGK}}(\mathbf{x}, t) = \frac{\Delta t}{\tau} (f_q^{\text{eq}}(\rho_f, \mathbf{U}) - f_q(\mathbf{x}, t)). \quad (5)$$

It features the relaxation time  $\tau \in (\frac{1}{2}, \infty)$  which determines the kinematic fluid viscosity  $\nu$  via

$$\nu = \left( \tau - \frac{\Delta t}{2} \right) c_s^2. \quad (6)$$

The forcing operator in Eq. (1) is used to incorporate external forces and can be written as

$$\mathcal{F}_q(\mathbf{x}, t) = \Delta t w_q \left[ \frac{\mathbf{c}_q - \mathbf{U}}{c_s^2} + \frac{\mathbf{c}_q \cdot \mathbf{U}}{c_s^4} \mathbf{c}_q \right] \cdot \mathbf{f}^{\text{ext}}, \quad (7)$$

with a constant force density  $\mathbf{f}^{\text{ext}}$  [44]. The cell local macroscopic velocity  $\mathbf{u}$  is then obtained via

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{U}(\mathbf{x}, t) + \frac{\Delta t}{2\rho_0} \mathbf{f}^{\text{ext}}, \quad (8)$$

and thus differs from the velocity  $\mathbf{U}$ , which is used to calculate  $f_q^{\text{eq}}$  and  $\mathcal{F}_q$  in Eqs. (3) and (7), respectively, by a shift depending on  $\mathbf{f}^{\text{ext}}$  [45].

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