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# Particle flow simulations with homogenised lattice Boltzmann methods

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ABSTRACT

An alternative approach to simulating arbitrarily shaped particles submersed in viscous fluid in two dimensions is proposed, obtained by adapting the velocity parameter of the equilibrium distribution function of a standard lattice Boltzmann method (LBM). Comparisons of exemplifying simulations to results in the literature validate the approach as well as the convergence analysis. Pressure fluctuations occurring in Ladd's approach are greatly reduced. In comparison with the immersed boundary method, this approach does not require cost intensive interpolations. The parallel efficiency of LBM is retained. An intrinsic momentum transfer is observed during particle–particle collisions. To demonstrate the capabilities of the approach, sedimentation of particles of several shapes is simulated despite omitting an explicit particle collision model.



## Introduction

Suspensions play an important role in many technical and even non-technical processes. Most often, suspensions are polydisperse, i.e., the solid objects submerged in the fluid differ in size, mass, or shape. Experiments demonstrate that non-uniformity crucially influences the dynamics of suspensions, in, for example, sedimentation, mixing processes, and nanomedicine applications, where non-spherical nanoparticles improve tumour targeting over spherical ones (Park et al., 2008). Many shape-dependent effects, such as drag, sedimentation behaviour, and even electrical properties of nanomaterials (Park et al., 2008), are still not fully understood and therefore in the focus of several research groups. With a deeper understanding, sophisticated models as well as numerical simulations could deliver highly valuable insights.

A great and so far unsolved challenge is to find an efficient approach that enables the dynamics of thousands or millions of differently and arbitrarily shaped objects to be predicted (Lu, Third, & Müller, 2015), and thereby be able to calculation the interaction between objects as well as with the fluid. Unfortunately this incurs enormous computational costs. The main aim of this paper is to contribute a new approach and a numerical scheme towards providing an accurate as well as efficient simulation for huge numbers of arbitrarily shaped particles.

To date, most approaches are limited to spherical particles or to a rather small number of arbitrarily shaped particles. In general, two main classes can be distinguished, first, Euler–Euler (EE) methods where a particle phase is described by a density distribution and modelled by a convection–diffusion equation and, second, Euler–Lagrange (EL) methods where the trajectories of a number of discrete particles are computed according to Newton's law of motion. In both cases, usually an incompressible Newtonian fluid is modelled by the Navier –Stokes equations. Recently proposed EE models, (e.g., John et al., 2009), are able to perform dynamics simulations for arbitrarily sized particles. The particle phase is modelled by a convection–diffusion-reaction equation with a balance equation for the particle size distribution. However, until now, only EE methods for spherical particle systems have been proposed.

EL methods can further be categorized as fixed-mesh or body-conformal-mesh methods, like the arbitrary Lagrangian–Eulerian (ALE) method (Hu, Joseph, & Crochet, 1992). Because of algorithmic complexity, as well as the high computational cost in re-meshing, the latter methods are limited to dynamics simulation of only a few particles. Such EL methods, where the objects are not resolved in the fluid, specify a drag force model enabling a two-way coupling of the fluid with the moving object. With it, a dynamics

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**Nomenclature**

| | |
|---|---|
| $c_\mathrm{D}$ | Drag coefficient |
| $c_\mathrm{L}$ | Lift coefficient |
| $d_k$ | Porosity |
| $d(\mathbf{x}, t)$ | A level-set function related to moving porosity |
| $D$ | Particle (sphere or cylinder) diameter |
| $D_{kl}$ | Distance between particles $k$ and $l$ |
| $D'_i$ | Distance from $\mathbf{X}_k$ to the closest point $\mathbf{X}'_k$ on the wall |
| $D(\mathbf{x}, t)$ | Denominator of $\mathbf{u}^\mathrm{B}(\mathbf{x}, t)$ |
| $E$ | Particle's kinetic energy |
| $f_i$ | Distribution functions for fluid particles |
| $f_{i*}$ | Momentum distribution in the opposite direction of $f_i$ |
| $f_i^\mathrm{eq}$ | Equilibrium distribution function |
| $\mathbf{F}_\mathrm{D}$ | Drag force |
| $\mathbf{F}_\mathrm{L}$ | Lift force |
| $\mathbf{F}_k$ | Total force acting on particle $k$ |
| $\mathbf{F}_k^\mathrm{F}$ | Hydrodynamic force acting on particle $k$ |
| $\mathbf{F}_k^\mathrm{pp}$ | Particle–particle interaction force |
| $\mathbf{F}_k^\mathrm{pw}$ | Particle–wall interaction force |
| $\mathbf{F}_k^\mathrm{g}$ | Gravitational force acting on particle $k$ |
| $h$ | Step size |
| $J_k$ | Particles' moment of inertia |
| $L_k$ | Half-edge length of cubical particles |
| $M_k$ | Particles' mass |
| $N$ | Resolution |
| $\mathbf{N}(\mathbf{x}, t)$ | Numerator of $\mathbf{u}^\mathrm{B}(\mathbf{x}, t)$ |
| $R_k$ | Radius of spherical particles |
| $R^\mathrm{P}$ | Radius of the circumscribed circle of all particles |
| $r_i^\mathrm{B}$ | Physical radius of the $i$-th particle |
| $R_i$ | Outer radius of a particle |
| $Re^\mathrm{P}$ | Particle's Reynolds number |
| $\mathbf{T}_k^\mathrm{F}$ | Torque |
| $\bar{\mathbf{u}}(\mathbf{x}, t)$ | Velocity |
| $\bar{\mathbf{u}}_k^\mathrm{P}(t)$ | Particles' velocity |
| $\mathbf{u}^\mathrm{F}(\mathbf{x}, t)$ | Macroscopic fluid velocity |
| $\mathbf{u}^\mathrm{F}$ | Fluid velocity |
| $\mathbf{u}^\mathrm{B}(\mathbf{x}, t)$ | Weighted average of the particle velocity |
| $\mathbf{u}^\mathrm{B}$ | Rigid-body velocity |
| $\mathbf{u}_k^\mathrm{P}(\mathbf{x}, t)$ | Sum of the translational velocity of the particle mass centre and the particle angular velocities |
| $\mathbf{u}_\mathrm{t}$ | Tangential velocity on cylinder boundary $S$ |
| $\mathbf{U}^\mathrm{P}$ | Particles' vertical velocity |
| $\mathbf{v}_i$ | Discrete mesoscopic velocities |
| $\mathbf{X}_k(t)$ | Particles' position (centre of mass) |
| $y_\mathrm{p}$ | Particle vertical position |
| $\tau$ | Relaxation time |
| $\nu$ | Fluid kinematic viscosity |
| $\rho^\mathrm{F}(\mathbf{x}, t)$ | Macroscopic fluid density |
| $\rho^\mathrm{P}$ | Particle density |
| $\varepsilon_\mathrm{h}$ & $\varepsilon$ | Smoothing parameter |
| $\gamma$ & $\gamma_w$ | Parameters in Eq. (10) |

*Acronyms*

| | |
|---|---|
| ALE | Arbitrary Lagrangian–Eulerian |
| BGK | Bhatnagar–Gross–Krook |
| DKT | Drafting–kissing–tumbling |
| EE | Euler–Euler |
| EL | Euler–Lagrange |
| EOC | Experimental order of convergence |
| FD | Fictitious domain |
| HLBM | Homogenised lattice Boltzmann method |
| IB | Immersed boundary |
| IBM | Immersed boundary method |
| LBM | Lattice Boltzmann method |
| MLUPS | Million lattice site updates per second |
| MEA | Momentum exchange algorithm |

simulation of millions of particles (cf. Tsuji, Yabumoto, & Tanaka, 2008) becomes feasible. However, the objects' shapes are not arbitrary but limited to rather simple primitives (cf. Vollmari, Jasevičius, & Kruggel-Emden, 2016). The most prominent fixed-mesh methods for fully resolved objects are immersed boundary (IB) (Peskin, 1972) and fictitious domain (FD) methods (Glowinski, Pan, Hesla, & Joseph, 1999; Glowinski, Pan, Hesla, Joseph, & Periaux, 2001). Both employ multiple grids, one Eulerian for the fluid phase and one Lagrangian for each particle. Each Lagrangian grid moves with its particle's velocity as the result of the computed hydrodynamics and other forces (e.g., gravity, collision), and the coupling back to the fluid is realised by sophisticated forcing schemes. In contrast to EE, EL methods in principle allow the simulation of arbitrary shapes (Nakayama & Yamamoto, 2005). However, to the best of our knowledge, there only exist dynamics simulations for single non-spherical particles (cf. Aidun, Lu, & Ding, 1998; Chen, Cai, Xia, Wang, & Chen, 2013; Eshghinejadfard, Abdelsamie, Janiga, & Thévenin, 2016; Huang, Yang, Krafczyk, & Lu, 2012; Kim & Choi, 2006; Lv, Tang, & Zhou, 2012; Rosén, Lundell, & Aidun, 2014; Suzuki & Inamuro, 2011; Swaminathan, Mukundakrishnan, & Hu, 2006; Xia et al., 2009), which may be because collision modelling for arbitrary-shaped particles is lacking (Aidun et al., 1998; Eshghinejadfard et al., 2016), computational demands are high, and implementations are complex (Swaminathan et al., 2006).

In recent years, lattice Boltzmann methods (LBMs) have evolved to be complete with classical tools in solving complex fluid flows problems. Since 1994 when Ladd used an EL method (Ladd, 1994a, 1994b) and most recently by an EE method (Trunk, Henn, Dörfler, Nirschl, & Krause, 2016), LBM has been shown to be able to simulate particulate flows. The explicit scheme, consisting of computationally localised colliding and streaming steps, allows highly efficient executions on massively parallel platforms (Henn, Thäter, Dörfler, Nirschl, & Krause, 2016; Krause, ThäTer, & Heuveline, 2013). Similar to Ladd, Götz, Feichtinger, Iglberger, Donath, and Rüde (2008) incorporated spherical particles by a boundary condition method and demonstrated its capability by simulating up to 150,000 particles. An IB method was introduced in an LBM context by Feng and Michaelides (2004, 2005) and further improved by Hu, Yuan, Shu, Niu, and Li (2014), Niu, Shu, Chew, and Peng (2006), and Wu and Shu (2009). Shi and Phan-Thien (2005) proposed an FD method for particulate flows in LBM, which was extended by Nie and Lin (2010, 2011). They all applied their methods for the dynamics simulation for spherical particles. Another promising EL fixed-mesh approach has been proposed by Nakayama and Yamamoto (2005). The smoothed-profile method models the boundaries of objects through a continuous transition between fluid and particle velocities. Later, the idea was introduced into LBM by Jafari, Yamamoto, and Rahnama (2011). In principle, the method allows the simulation of particles of arbitrary shape. However, until now, it has not been applied to particles of other shapes.

In this work, an alternative approach is proposed, referred to as the homogenised lattice Boltzmann method (HLBM). It extends the porous media model, introduced into LBM by Spaid and Phelan (1997), towards one which enables the simulation of moving porous media. We apply the general HLBM for the simulation of moving particles of arbitrary shape. To avoid pressure fluctuations, the local porosity coefficient is used as a smoothing parameter, sim-

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