Drag Force Simulations of Particle Agglomerates with the Lattice-Boltzmann Method

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Abstract

In this work we show, that the Lattice Boltzmann method is capable of calculating the drag force on spheres with a sufficient accuracy. The main interest lies on laminar flows around nano particle agglomerates. To give an overview over the simulated force accuracy the results are compared with analytical solutions. Thereby the benefit from curved boundary treatments such as [YD03] and [PL03] is taken into account. Through the use of curved boundary treatments the lattice radius of the spheres can be reduced and thus smaller domain sizes can be used with the same force accuracy. Further more, results for complex agglomerates are presented and compared to solutions of the Stokesian Dynamics approach [AS01].

1 Introduction

In the field of measurement engineering and also in particle technology the interaction of particle agglomerates with the surrounding fluid is an important research area, as there are often no analytical solutions for the estimation of the forces acting upon particle agglomerates. Thus one solution to overcome this problem is to solve the fluid flow with a numerical approach and to calculate the forces acting upon the agglomerates with information from the simulation. Here the fluid flow has been simulated with the Lattice Boltzmann method (LBM), which is an alternative method to simulate computational fluid dynamics. It can be shown that the LBM is able to efficiently compute an approximation of the Navier Stokes Equations. The simulated forces have been calculated with the momentum exchange method, which is unique to the LBM. The intention of this work is to examine if the LBM is capable of calculating the drag force on spheres with a sufficient precision.

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2 The Lattice Boltzmann Method

The Lattice Boltzmann method is an approach to solve computational fluid dynamic(CFD) problems, which has gained a great deal of popularity in recent years. Most traditional CFD solvers obtain the macroscopic parameters, like the velocity and pressure, by solving the incompressible Navier-Stokes (NS) equations with finite differences, finite volumes or finite elements. With the LBM the macroscopic parameters of the fluid result from the propagation and collision of particles, which are represented by averaged particle distribution functions. For further details on the LBM method see [DYS03] [Fei05].

3 Boundary conditions

One of the current research topics is the boundary treatment in the LBM. For this work the obstacle boundaries are of great importance, as they directly determine the flow near the obstacles, which is used to calculate the force acting upon obstacles. It thus determines the precision of the simulated force values. The standard boundary treatment for solid walls in the LBM is the so called bounce back scheme (see [DYS03]). With this method curved boundaries have to be approximated by stair steps, what also effects the precision of the particle distributions near a curved obstacle. Another investigated possibility is to use curved boundary treatments. The used curved boundary schemes were developed by Yu et al. [YD03] and Lallemand et al. [PL03]. The idea of all these schemes is to interpolate the flow near the wall and thereby incorporate the real position of the curved boundary.

4 Drag force calculation

A crucial topic in fluid dynamics is the evaluation of the acting force on a body in a fluid. As there is no analytical solution for the calculation of the drag force on particle agglomerates and even approximations can only be done for spheres, the simulation of the drag force on particle agglomerates is still a challenge. For a single sphere there exists an analytical solution in laminar flows(Stokes flow):

$$\vec{F}_D = 3\pi \, \eta \, d \, \vec{u}_{rel} \tag{1}$$

$$\vec{u}_{rel} = \vec{u}_{fluid} - \vec{u}_{particle} \tag{2}$$

where η is the dynamic viscosity and $\vec{u}_{rel}$ is the approach velocity. These formulas are used in the result Section to estimate the accuracy of the momentum exchange approach. The momentum exchange approach is unique to the LBM, as it makes use of the particles moving back and forth from the surface of obstacles contained in the fluid, which is information that is not available for traditional NS solvers.

5 Results

5.1 Single sphere tests

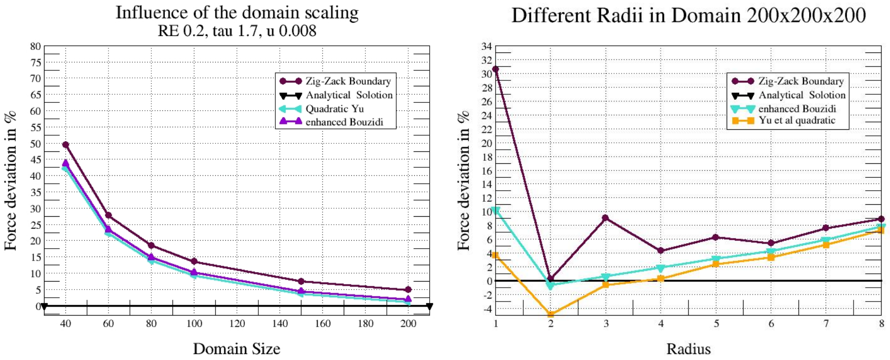

Figure 1: On the left the comparison between the boundary methods for different domains is shown and the right chart the influence of the radius on the force accuracy is depicted. In both figures the derivation of the simulated force from the analytical solution is depicted in per cent

A first comparison of the simulated force and the analytical solution is given in Figure 1: a sphere is placed in the middle of various cubic domains with a constant in-/outflow. The Reynolds number was set to 0.2 and the radius of the sphere was set to 5 lattice units. This results in a reasonable approximation of the sphere, which will be shown below. The force is evaluated for all boundary methods from Section 2 and the analytical solution is determined with Eq. 1. The size of the domain has a huge effect on the accuracy of the force, but this has been expected as the analytical solution uses an infinitely large fluid region. Depending on the used scheme the force deviation from the analytical solution is reduced from about 50% to about 5%, when the domain size is increased from 40 to 200 in this test case. The difference between the curved boundary treatments and the zigzag boundary conditions is in this test case about 3-4% and it is fairly constant for all domain sizes. Thereby the Yu schemes results are slightly lower, than the ones of the Bouzidi scheme. However, the difference between the curved treatments, lies only within one 1 %, thus the accuracy gain between standard no-slip and curved boundary treatment is larger than the difference between the curved boundary treatments.

5.2 Influence of the radius in various domains

In the right chart of Figure 1 spheres with different radii are set in the middle of a 200^3 domain under the same conditions as in Section 5.1. What can be seen there, is that for

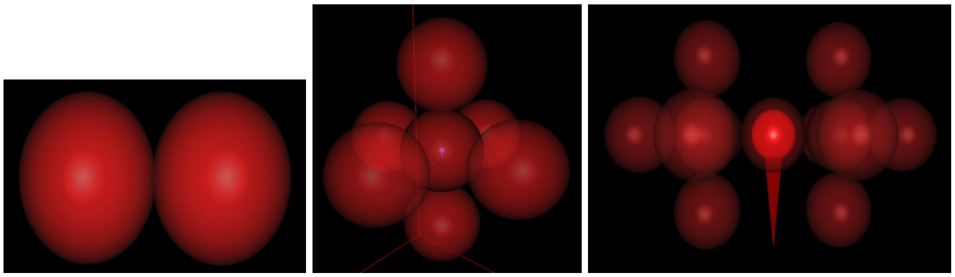

Figure 2: Three nano particle agglomerates

higher radii the deviation of the force from the analytical solution is increasing in all domains. Furthermore the zig-zag solution is approaching the curved boundary solutions. For a radius of eight the difference is only about 1-2%. This has been expected as the accuracy of the approximation improves with higher radii. The graph over the different radii for the zig-zag boundaries isn't straight for all domains, but rather jaggy and the magnitude of the jumps decreases with larger radii. These leaps result from the approximation of the sphere through cubes. The graphs for the curved boundary treatments are smoother. This is due to the better approximation of the sphere through the offsets. Still, for very small radii (1-2) even the curved boundaries can't compensate the bad approximation of the sphere. Good approximation results are achieved for a radius around 4 for the curved boundaries and for a radius of 6 for the zig-zag boundaries.

6 Particle agglomerates

In this section the drag force calculation on particle agglomerates is investigated. Therefore the force on three nano agglomerates has been simulated (see Figure 2). The flow is again laminar (RE<0.25) and for all LBM results the quadratic Yu scheme has been used. The force results have been compared to the results gained by the Stokesian Dynamics method(SD)[AS01]. For this comparison the simulated forces have been normalized by a division with the analytical solution of a single sphere (for further details see [Fei05]).

6.1 Tests with a Doublette

The Doublette agglomerate consists of two identical spheres, which are connected at the midpoint of the fluid domain(see left of Figure 2). The drag force on the Doublette has been calculated for four upstream directions. In the tabular below it can be seen, that the norm of the simulated force is greatest when the flow streams at the front of the Doublette. This was expected, as in this case the flow sees the largest surface area.

Drag Force	LBM	SD
Front	1.395	1.502
45°	1.358	1.416
Side	1.261	1.325

6.2 Symmetric star

The first agglomerate is a symmetric star consisting of 7 spheres (see mid image of Figure 2), which are all the same size. For the simulation a radius of three has been chosen, thus the maximum diameter of the structure is 18. The domain size was 300^3, the inflow velocity was set to $(0, -0.0052, 0)$ and τ to 1.9. Thus the resulting RE for the setup is 0.2.

Single star	LBM	SD
Drag Force	(0 2.39185 0)	(0 2.70303 0)

After the normalization the force result the SD value is about 31% larger than the solution with the Yu scheme. For an estimation of the domain border error, the force derivation has been determined for a sphere with the the maximum diameter of the agglomerate. As the influence of the border is larger the closer the agglomerate gets to the border, the case of a sphere with the maximum diameter of the agglomerate represents the maximum border influence for this agglomerate. Thus the maximum border influence for the simulated agglomerate should be less than 8.62%.

6.3 Symmetric double star

The symmetric double star consists of 13 spheres with a radius of 3.(see right image of Figure 2) The maximum diameter is 30 and the domain size has been set to 300, thus the border influence is larger than for the single star. The Yu scheme result is again lower than the one of the zig-zag boundaries. As can be seen in the tabular below, the results from the alternative method are lower, then the results form the LBM simulation. This may be due to the fact, that the force derivation from the correct solution for this agglomerate is larger than for the single star, due to the larger border influence.

Symmetric double star	LBM	SD
Drag Force	(0 3.98777 0)	(0 3.55716 0)

7 Conclusion

It was shown in this work, that the Lattice Boltzmann Method is able to simulate the drag force on particle agglomerates with sufficient accuracy. The influence of the lattice size of the spheres was examined and it turned out that for small radii (1-4) the force accuracy depends on the position of the particle in the grid. For larger radii this dependence is reduced. However for the drag force calculation with large radii the domain sizes have to be strongly increased to gain a benefit from the better approximations of the particle.
Additionally several curved boundary conditions have been investigated in this thesis and it turned out that these are able to give a better approximation of the spherical particles and thus can be used to reduce the lattice size of the particles. As for the accuracy improvement of the different curved boundary conditions, they are all quite similar compared to the difference between zig-zag and curved boundaries.
Furthermore the drag force is usually determined in infinitely large fluid domains and thus the domain size turned out to be a crucial factor for the force accuracy in laminar flows, leading to the drawback of the current implementation: time and memory consumption, since for large particle agglomerates simulations can require several GByte of main memory. The maximum domain size, which could be simulated with the currently available hardware for this work was 350^3, which is too small for the demands of real world problems. This shows the necessity for optimizations, such as grid adoptivity to enable the simulations with larger domains and reduce the runtime of the simulations.

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