Simulation of moving Nano-Particles with the Lattice Boltzmann Method in 3D

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Abstract

The following work presents a way to simulate the nano-particle behavior in a flow by coupling the Lattice Boltzmann Method to a rigid body physics engine. By extending the basic fluid simulation for the treatment of curved particle surfaces and by a force interaction method, the fluid forces acting on the nano-particles can be calculated. With this force interaction between the fluid and the particles and the use of the rigid body physics engine, the movement and collision behavior of nano-particles in a flow can be simulated. Additionally, this coupled simulation system is able to calculate the internal particle forces in the connections between sintered particles, which could break due to the forces of a shear flow. Therefore a prediction of possible break-ups becomes possible.

1 Motivation

The application of nano-particles in the production of numerous everyday life products has become an important factor for nearly every company. For example the transparency of plastic foil is strongly influenced by the structure and structural behavior of the used nano-particles. Without the application of nano-particles, the foil wouldn't have its transparency and only with certain particles the foil is resistant to strain. In the field of particle technology, the question of the structure and structural properties of nano-particles is essential for the prediction of the particle behavior. Due to the complex structure of these nano-particles, the analytical examination is limited to only very simple structures. The numerical simulation is one way to efficiently examine the structure and behavior of the nano-particles and therefore create new products faster and less costly.

2 Particles and Agglomerates

The nano-particles in this simulation can either be particles or agglomerates. Particles are an unbreakable compound of atoms and molecules and are of arbitrary shape and mass.

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The connection to other particles results in agglomerates, which are of arbitrary and often very complex structure, but breakable in certain contact points.

Since the structure of most particles is of a spherical character and their behavior in a flow resembles the behavior of a sphere, these particles are often approximated by spheres. Although this is an abstraction from the real world structure, experiments show, that the particle behavior in a flow is not tempered. The agglomerates in this simulation use this approximation to the real world structure: agglomerates consist of several spherical bodies, which replace the physical structure of the particles. These spheres are connected by point contacts or contact areas for overlapping particles. All particles are of arbitrary radius and of arbitrary mass, which is used as a point mass in the center of the spherical body. For all particles, which have a contact to other particles, a connection is simulated. In order to predict break-ups, the forces acting on these connections are calculated.

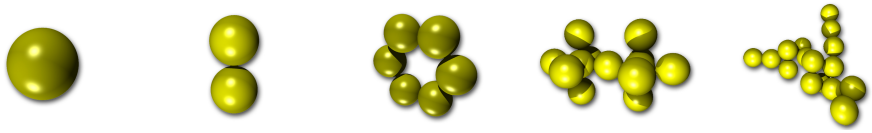

Figure 1: Possible agglomerates for the moving particle simulation

3 The Lattice Boltzmann Method

In contrast to the classical, macroscopic Navier-Stokes (NS) approach to simulate fluids, the Lattice Boltzmann Method (LBM) uses a mesoscopic simulation model. Instead of directly solving the macroscopic fluid quantities like the velocity and the pressure, the movement of the fluid particles is modeled. The choice of using the LBM for the fluid simulation is very good for this simulation due to the kinetic origin of the LBM, which is based on the Boltzmann equation. This makes the force interaction with the moving particles and particle agglomerates particularly easy. For detailed information about the Lattice Boltzmann Method, see [1], [2] or [3].

4 Two System Simulation

In order to simulate moving particles and agglomerates in a flow, the interesting problem of coupling two independent simulation systems occurs: the LBM, which simulates the fluid behavior, has to be coupled to a rigid body physics engine, which simulates the correct rigid body movements of particles and agglomerates. In this case, the open source rigid body physics engine ODE was chosen [5]. The first coupling step from the physical simulation to the fluid simulation is to determine the geometry of the particles and particle agglomerates in the fluid simulation. Due to the spherical character of the particles used in this simulation, the LBM has to be extended with the treatment of curved boundaries.

Without this extension, the fluid simulation would suffer stability problems especially for higher Reynolds' numbers. Detailed information about the boundary treatments for the LBM can be found in [2], [3] and [4]. The second coupling step from the fluid simulation back to the physical simulation is the force interaction between the fluid and the particles and agglomerates. Due to the kinetic origin of the LBM, this extension is efficiently solved by the momentum exchange method (see [2] and [3]). With the fluid forces acting on the particles and agglomerates, the rigid body physics engine can now simulate the physically correct movements of the particles and agglomerates. Using the calculated fluid forces, further external forces like for example gravity and the particle movements, the internal forces in each connection between sintered particles can be calculated. With this information, possible break-ups and ruptures in the structure of agglomerates can be determined. For a full explanation of the extended LBM algorithm and for detailed insight into the necessary extensions, see [2].

5 Results

In order to demonstrate the capability of the moving nano-particle simulation, three different scenarios are chosen. The first simulation result demonstrates the accuracy of the simulation, whereas the second and third scenario show the ability to simulate complex agglomerates.

One of the possible test scenarios for a comparison between analytical results and the moving particle simulation is to compare the sinking velocity of a heavy particle. A particle with a density of $2.0\frac{kg}{dm^3}$ (lattice density of 2) is put in the upper half of a box completely filled with fluid with density $1.0\frac{kg}{dm^3}$ (lattice density of 1). The only driving force in this setup is the gravity acceleration. Then the sinking velocity measured in the simulation is compared to the analytical value calculated as

$$v = \frac{2gr^2 \cdot (\rho_P - \rho_F)}{9\eta}, \tag{1}$$

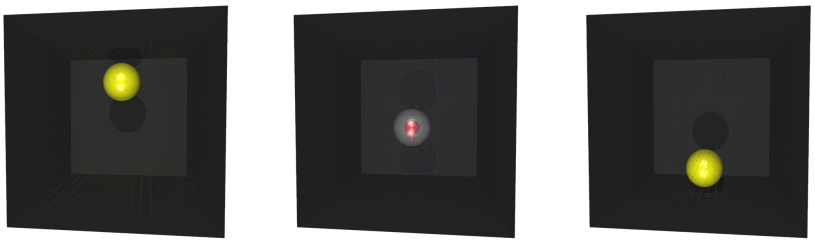

Figure 2: Sinking particle for the comparison between analytical results and the simulation

where g is the gravity acceleration of $9.81\frac{m}{s^2}$, r is the particle radius, ρ_P is the particle density, ρ_F the fluid density and η is the dynamic fluid viscosity. The analytical solution

calculated with Equation (1) is $v = 5.45 \cdot 10^{-3} \frac{m}{s}$ for a particle with a physical radius $r = 5 \cdot 10^{-5} m$ and a lattice radius of $r = 5$. Figure 3 shows the simulation results for the sinking velocity and the total force acting on the sinking particle for a simulation in a 60^3 domain. Although slightly larger than the analytical result, the sinking velocity agrees with the analytical value. The difference can be explained by the periodic force fluctuations caused the momentum exchange method in combination with moving particle surfaces (see [2]).

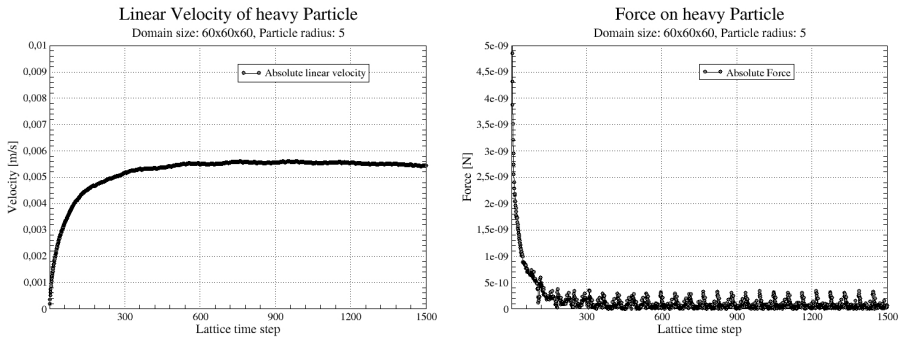

Figure 3: Simulation results for the sinking particle simulation

The second simulation puts a symmetric 13-particle dual star agglomerate in a shear flow, which results from a flow to the right in the upper half and a flow to the left in the lower half of the domain. Due to the resulting shear forces, the agglomerate starts rotating around its center of mass in the center particle due to its symmetric structure (see Figures 4). For the simulation, a physical cell size of $5 \cdot 10^{-5} m$ and a physical particle radius of $4 \cdot 10^{-4} m$ were chosen. This results in a lattice radius of 8 for each particle. The domain size was set to 120^3. Figure 5 shows the resulting connection forces for both connections of the center particle. Since the agglomerate is rotating around the y-axis, the force in y-direction is zero, whereas the force in x- and z-direction show the expected sinus behavior due to the rotational movement. It can also be seen that the force in both connections is exactly the inverse of each other. However, the force shows obvious fluctuations, as in the first simulation scenario, which is again caused by the momentum exchange method. Unfortunately, this agglomerate is too complex to compare the simulation results to analytical calculations. However, as the first simulation scenario has demonstrated, credible results can be achieved with this simulation. Furthermore, the simulation shows no stability problems and very smooth and credible movements. Therefore, this simulation could be used in order to estimate break-ups in the agglomerate structure.

In the third simulation, the dual star agglomerate is replaced by a complex 16-particle agglomerate with unsymmetric structure. As in the second simulation, no comparison

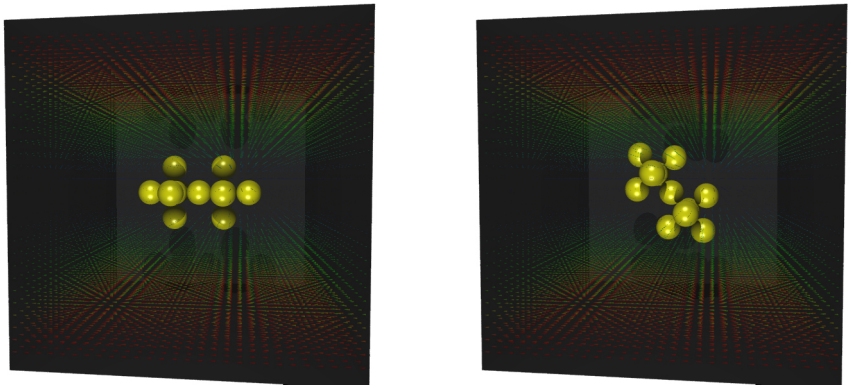

Figure 4: Rotating symmetric 13-particle agglomerate in a shear flow

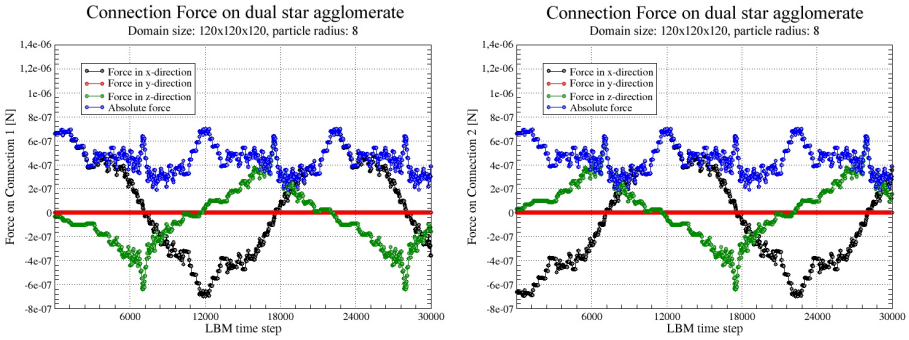

Figure 5: Internal forces for both center connections

to analytical results can be performed, but again, no stability problems occur and the movement of the agglomerate is smooth and credible.

6 Conclusion

The investigation of the flow behavior of nano-particles can efficiently be performed by the numerical simulation approach presented in this work. By extending the LBM with a treatment for curved boundaries and a force interaction method between the fluid and the nano-particles and by coupling this fluid simulation to a rigid body physics engine, an accurate simulation of moving agglomerates can be implemented. This simulation is also able to calculate the connection forces between several sintered particles and therefore predict connection break-ups.

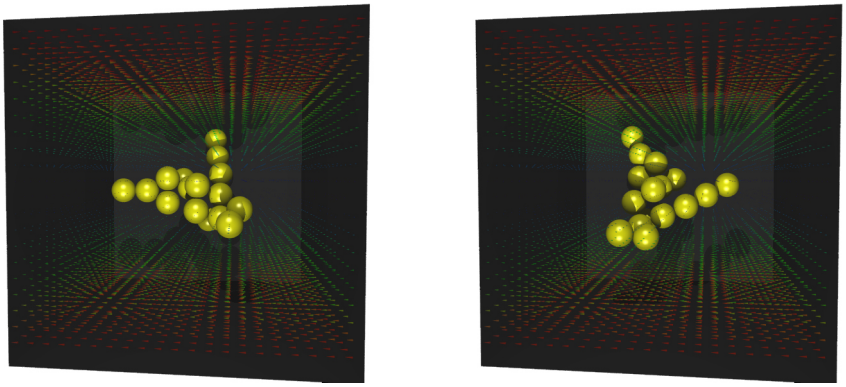

Figure 6: Rotating 16-particle agglomerate in a shear flow

However, in some simulations, the accuracy of the simulation results still has to be improved. For example, the momentum exchange approach could be extended by a finite volume calculation in order to reduce the force fluctuations. The accuracy of the simulated results can also be improved by locally increasing the grid resolution with grid refinement techniques and a deeper understanding of the influence of the LBM simulation parameters and boundary condition influences.

References

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[5] Official Open Dynamics Engine (ODE) Homepage: http://www.ode.org