Available online at www.sciencedirect.com
ScienceDirect
Computers and Mathematics with Applications 55 (2008) 1461–1468
An International Journal
computers & mathematics
with applications
www.elsevier.com/locate/camwa

Simulation of moving particles in 3D with the Lattice Boltzmann method

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Abstract

The following paper presents a way to simulate the behavior of particle agglomerates in a fluid flow by coupling the Lattice Boltzmann Method to a rigid body physics engine. By extending the basic algorithm by a fluid/particle force interaction method, the hydrodynamic forces acting on the particles can be calculated. By the use of this force interaction between the fluid and the particles and by the use of the rigid body physics engine, the movement and collision behavior of particles in a flow can be simulated. Additionally, this coupled simulation system is able to simulate the internal particle forces in the connections between sintered particles, which could break due to the forces and torques of a shear flow. This permits a prediction of possible break-ups or structural displacements.

Keywords: Lattice Boltzmann method; Curved boundaries; Force interaction; Rigid body physics; Particles; Agglomerates

1. Introduction

In the field of particle technology, knowledge about the behavior of complex particles in a flow is essential to predict the properties of the final products containing these particles. However, the behavior of the particles is dependent on their structure. Due to the complex structure of these particles, the analytical examination is limited to only very simple structures. Numerical simulation is one way to efficiently examine the structure and behavior of the particles and therefore create products faster and at lower cost.

This paper proposes to simulate particles and particle agglomerates in a flow by coupling a rigid body physics engine to a Lattice Boltzmann fluid simulation. This new approach is to our current knowledge the first attempt to simulate moving particle agglomerates in a flow that also offers the possibility to simulate arbitrarily complex agglomerates and to calculate contact forces and torques. These can be used to simulate break-ups or structural displacements within the agglomerates. We achieve this by combining several extensions for the fluid simulation like the treatment of moving curved boundaries with the scheme of Yu et al. [1] and a fluid/particle force interaction method with the momentum exchange method of Ladd [2]. An overview of these techniques can be found in [3]. The simulations in Section 5 will show that our approach yields stable and accurate results of arbitrarily complex agglomerates.

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doi:10.1016/j.camwa.2007.08.022

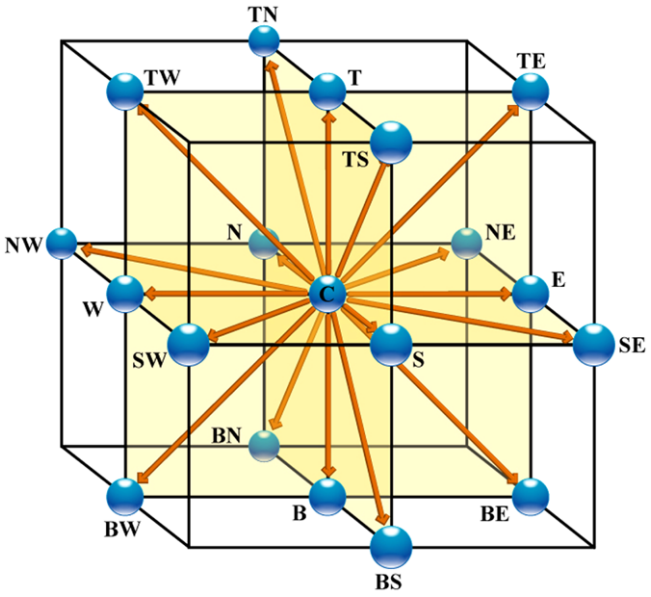

Fig. 1. The D3Q19 model for the 3D LBM.

2. 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 [4]. Instead of directly solving the macroscopic fluid quantities, such as velocity and pressure, the movement of fluid particles is modeled. The fluid domain is discretized in uniform Cartesian cells. Each cell holds a fixed number of distribution functions, which represent the number of fluid particles moving in these discrete directions. For this work, the most popular model for the 3D case, the D3Q19 model, which consists of 19 distribution functions, has been used. This model is illustrated in Fig. 1.

The distribution functions are calculated by solving the Lattice Boltzmann equation (LBE), which is a special discretization of the kinetic Boltzmann equation. Based on the Bhatnagar–Gross–Krook (BGK) model, the update of the distribution functions can be formulated as in Eq. (1):

$$f_\alpha(\mathbf{x}_i + \mathbf{e}_\alpha \delta t, t + \delta t) - f_\alpha(\mathbf{x}_i, t) = -\frac{1}{\tau}[f_\alpha(\mathbf{x}_i, t) - f_\alpha^{(\mathrm{eq})}(\mathbf{x}_i, t)], \tag{1}$$

where δt denotes the lattice time step, $\delta \mathbf{x} = \mathbf{e}_\alpha \delta t$ denotes the lattice cell size, τ denotes the lattice relaxation time, $\mathbf{e}_\alpha$ is the discrete lattice velocity in direction α, and $f_\alpha^{(\mathrm{eq})}$ is the equilibrium distribution (see Eq. (4)). Eq. (1) is usually solved in two steps:

$$\tilde{f}_\alpha(\mathbf{x}_i, t + \delta t) = f_\alpha(\mathbf{x}_i, t) - \frac{1}{\tau}[f_\alpha(\mathbf{x}_i, t) - f_\alpha^{(\mathrm{eq})}(\mathbf{x}_i, t)] \tag{2}$$

$$f_\alpha(\mathbf{x}_i + \mathbf{e}_\alpha \delta t, t + \delta t) = \tilde{f}_\alpha(\mathbf{x}_i, t + \delta t). \tag{3}$$

Eq. (2) is called the collide step. This step models various fluid particle interactions like collisions and calculates new distribution functions according to the distribution functions of the last time step. It also models the equilibrium distribution functions, which are calculated with Eq. (4).

$$f_\alpha^{(\mathrm{eq})} = w_\alpha \cdot \rho \cdot \left[1 + \frac{3}{c^2}\mathbf{e}_\alpha \cdot \mathbf{u} + \frac{9}{2c^4}(\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{3}{2c^2}\mathbf{u} \cdot \mathbf{u}\right]. \tag{4}$$

In this equation, w_α is a weighting factor depending on the LBM model used, ρ is the lattice fluid density, and $\mathbf{u}$ is the lattice fluid velocity.