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Measurements of wall shear stress with the lattice Boltzmann method and staircase approximation of boundaries

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ABSTRACT

We analyze the accuracy of wall shear stress measurements in lattice Boltzmann simulations that are based on a voxel representation of the geometry and staircase approximation of boundaries. Such approximations are commonly used in the context of lattice Boltzmann simulations, because they favor the use of simple and highly efficient data structures. We show on several two- and three-dimensional simulations that this low-order approximation of the boundary affects the accuracy of wall shear stress measurements in areas directly adjacent to the wall. A few lattice nodes apart from the wall, the accuracy is however largely improved, and can be considered to be compatible with the overall accuracy of a simulation at a given coarseness level of the grid. This result is interpreted as a justification for the use of walls with staircase shape, even in simulations with high expectations regarding the level of accuracy. Furthermore, we propose a novel method for establishing the direction of the wall normal, a quantity which is required for the computation of the wall shear stress. With this method, the wall normal is computed from local data that is extracted from the results of the fluid flow simulation. Owing to the nature of the flow dynamics, which tends to smooth out the asperities of the wall, the information on the wall orientation obtained in this way is observed to be of high quality.

1. Introduction

Over the last years, the lattice Boltzmann method has established itself as a tool for numerical simulation of fluid flows [1,4–6]. One major advantage of the method is the possibility to incorporate complicated boundary conditions relatively easily. Since the method works on a regular rectangular grid, no complex mesh generation is necessary, and simulation setup for complicated geometries can be automatized.

A simple approach to handle complex boundaries is to approximate them by a staircase shape, and to use a bounce-back scheme (see for instance [5,11]) to implement no-slip boundary conditions. More accurate schemes exist, which resolve the actual boundary location with sub-grid resolution, e.g. the method proposed by Bouzidi et al. [3]. However, these schemes require non-local surface smoothing processes to generate sub-grid boundary locations from voxel data. This might be unacceptably expensive when simulating systems with time-dependent boundary locations, where the smoothing process would have to be performed every time the type of a voxel cell changes. An example is a boundary changed by deposition and erosion of materials transported by the fluid. The inevitable non-locality of the smoothing process is particularly unfavorable when running simulations on parallel computers. We also point out that it would be interesting to compare the bounce-back approach used in the present paper with a recently published local boundary condition presented in [7].

Hence, the staircase plus bounce-back approach to the problem of complicated boundaries is worth being considered due to its technical advantages, if the desired accuracy allows it.

This work has been motivated by ongoing research on coupling a lattice Boltzmann fluid solver with other models to simulate the interaction of hemodynamics and physiological processes in artery disease. It is now widely accepted that wall shear stress, i.e. the shear stress exerted by the viscous fluid as it moves along the artery walls, acts as a factor for physiological processes in the artery wall tissue [10,2]. However, the influence is not yet quantitatively precisely understood, thus wall shear stress measurements would not need to be overly accurate as input to the other models. One purpose of this paper is to investigate whether acceptably accurate wall shear stress measurements can be obtained when staircase approximation of boundaries and bounce-back scheme are used.

Our second intent is to propose a method for purely local measurements of the wall shear stress, allowing for easy and efficient parallel implementation. To compute wall shear stress, the local deviatoric stress tensor and the boundary normal vector must be known. The former is locally available in the lattice Boltzmann

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method, on all nodes close to the boundary, without need for spatial interpolations. Determination of the boundary normal, however, would customarily require a non-local procedure, because the staircase-approximated boundary offers too little information. We propose a technique to detect the boundary normal direction locally, using information from the fluid field. The method works well for the 2d and 3d benchmark cases tested. It should be mentioned that there exists another way of computing the wall normal in a voxelized geometry, which consists in solving a Poisson equation within the fluid domain [9]. The advantage of the method in the present paper is that it requires no additional equation to be solved, and is therefore both simpler and more efficient to implement. The advantage of the approach presented in [9] is that, first of all, it offers a means of computing the distance to the wall in a general geometry, and second, it remains valid at a larger distance from the wall, because the Poisson equation lacks a convective term which could spoil the accuracy of the calculation.

2. Theoretical background

2.1. Lattice Boltzmann method

Lattice Boltzmann models simulate the dynamics of particle distribution functions in a discretized phase-space.

The continuous space of positions is represented by the discrete set of nodes of a regular grid, with equal spacings δx in all directions. Similarly, the space of velocities is represented by a discrete set of q vectors $\vec{c_i}$, which are chosen such that the neighbors of a lattice node $\vec{x}$ are found at positions $\vec{x}+\delta t\,\vec{c_i}$, where δt is the discrete time step of the model.

Lattice topology is therefore defined by the set of velocities, and a d-dimensional lattice with q velocities is commonly referred to as a *DdQq* lattice.

Given the discretization of position and velocity space, the state of the simulation is completely defined by the values of q particle distribution functions f_i on each lattice node.

Hydrodynamic variables are defined as moments of the particle distribution functions. In particular, density ρ and momentum $\rho\vec{u}$ are computed as zeroth- and first-order moments:

$$\rho = \sum_i f_i, \quad \rho\vec{u} = \sum_i f_i \vec{c_i}\,. \tag{1}$$

The relation of the second-order moment

$$\mathbf{\Pi} = \sum_i f_i \vec{c_i}\,\vec{c_i} \tag{2}$$

to the hydrodynamic variables is explained below.

The dynamics of the particle distribution functions is governed by the lattice Boltzmann equation. When written in a system of lattice units where $\delta x = 1$ and $\delta t = 1$, it reads

$$f_i(\vec{x}+\vec{c_i}, t+1) = f_i(\vec{x}, t) + \Omega_i(\vec{x}, t). \tag{3}$$

This can be formulated as two steps, reflecting its practical implementation. First, the collision operator Ω is applied locally on all lattice nodes:

$$f_i'(\vec{x}, t) = f_i(\vec{x}, t) + \Omega_i(\vec{x}, t). \tag{4}$$

The post-collision distribution functions f_i' are then propagated to neighboring lattice nodes determined by the corresponding velocity vectors:

$$f_i(\vec{x}+\vec{c_i}, t+1) = f_i'(\vec{x}, t). \tag{5}$$

The collision step is strictly local, while the streaming step involves nearest neighbors.

In the commonly used lattice Boltzmann BGK model, the collision operator describes a relaxation of the particle distribution functions towards a local equilibrium:

$$\Omega_i = -\omega(f_i - f_i^{eq}(\rho, \vec{u})). \tag{6}$$

Here, ω is a relaxation frequency, and the local equilibrium f_i^{eq} depends only on ρ and $\vec{u}$.

By means of a multi-scale analysis, it can be shown that the lattice Boltzmann BGK model recovers the Navier–Stokes equations for a weakly compressible fluid (see for instance [5,6]). This analysis is not performed in detail here.

The key idea is to expand the lattice Boltzmann equation into a truncated Taylor series, and expand the particle distribution functions into a power series of a small parameter ϵ, often identified with the Knudsen number of the flow:

$$f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \mathcal{O}(\epsilon^2). \tag{7}$$

$f^{(0)} = f^{eq}$ is the equilibrium distribution, while the higher-order terms form the off-equilibrium part of the distribution. Off-equilibrium moments can be defined in analogy to Eqs. (1) and (2), replacing f_i with $f_i^{(n)}$. It can be shown [6] that the tensor $\mathbf{\Pi}^{(1)}$ is related to the strain rate tensor $\mathbf{S}$:

$$\mathbf{\Pi}^{(1)} = -\frac{2c_s^2\rho}{\omega}\mathbf{S}, \tag{8}$$

where S is defined as:

$$\mathbf{S} = \frac{1}{2}((\nabla\vec{u}) + (\nabla\vec{u})^t). \tag{9}$$

For practical purpose, $f_i^{(1)}$ is approximated as $f_i - f_i^{eq}$ and Eq. (8) implies that

$$\mathbf{S} = -\frac{\omega}{2c_s^2\rho}\mathbf{\Pi}^{(1)} = -\frac{\omega}{2c_s^2\rho}\sum_i (f_i - f_i^{eq})\vec{c}_i\vec{c}_i. \tag{10}$$

2.2. Bounce-back boundary conditions

To simulate flows in finite domains, one has to implement boundary conditions at certain nodes. After the streaming step, the values of some particle distribution functions are unknown at boundary nodes, since the corresponding neighbor nodes lie outside the fluid. Implementing a boundary condition amounts to define the values of the unknown distribution functions in a manner consistent with the dynamics of the model.

The easiest approach to implement a no-slip boundary condition is the so-called bounce-back scheme [5,11]. Particle distributions arriving at a boundary node from neighbor nodes inside the fluid are reflected back in the direction they came from. The scheme is obviously cheap and easy to implement. It fails, however, to resolve boundary locations at a scale smaller than the lattice spacing δx, since the no-slip condition is always satisfied in the middle of a link between two neighbor nodes.

2.3. Measuring wall shear stress and boundary normal

Wall shear stress is the force per unit area that is exerted by a moving viscous fluid on a solid boundary. In the following, Greek indexes denote spatial coordinates. Summation over any pair of identical Greek indexes is assumed. The total stress tensor for the fluid is

$$T_{\alpha\beta} = -p\cdot\delta_{\alpha\beta} + \sigma_{\alpha\beta}, \tag{11}$$

where p denotes pressure, $\delta_{\alpha\beta}$ is the Kronecker symbol and $\sigma_{\alpha\beta}$ denotes the contribution from the viscous forces. The stress on some boundary surface element with unit normal vector $\vec{n}$ is $T_{\alpha\beta}n_\beta$, and