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Evaluation of Pressure Boundary Conditions for Permeability Calculations Using the Lattice-Boltzmann Method

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Abstract. Lattice-Boltzmann (LB) simulations are a common tool to numerically estimate the permeability of porous media. For valuable results, the porous structure has to be well resolved resulting in a large computational effort as well as high memory demands. In order to estimate the permeability of realistic samples, it is of importance to not only implement very efficient codes, but also to choose the most appropriate simulation setup to achieve accurate results. With the focus on accuracy and computational effort, we present a comparison between different methods to apply an effective pressure gradient, efficient boundary conditions, as well as two LB implementations based on pore-matrix and pore-list data structures.

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1 Introduction

The lattice-Boltzmann (LB) method is a numerical scheme that is able to simulate the hydrodynamics of fluids with complex interfacial dynamics and boundaries [1–6]. Its popularity stems from the broad field of possible application and a fair implementation effort compared to other CFD methods. Unlike schemes that are based on a discretization of the Navier-Stokes equations and therefore represent balance equations at the continuum level (macroscopic), the LB method represents the dynamics at mesoscopic level by solving the discretized Boltzmann equation.

There is an increasing interest in the LB method for simulation of flow in complex geometries since the end of the 1980's [7] when hydrodynamic simulation methods

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were dominated by finite element schemes that solved the Stokes equation [8,9]. With the advent of more powerful computers it became possible to perform detailed simulations of flow in artificially generated geometries [10], tomographic reconstructions of sandstone samples [11–15], or fibrous sheets of paper [16]. An important property estimated using the LB method in those geometries is the permeability [17] and since the porous structure has to be well resolved in order to obtain valuable results, a large computational effort as well as large amounts of memory are required. Therefore, it is important to develop very efficient simulation paradigms.

Different alternative simulation setups have been proposed for permeability estimation which differ in the computational domain setup, boundary conditions (BC), how the fluid is driven, or how an effective pressure gradient is being estimated. Further possible differences include the choice between single relaxation and multirelaxation time lattice Boltzmann implementations or data structures based on a 3D array containing the whole discretized simulation volume including rock matrix and pore space (pore-matrix) in contrast to data structures limited to a connected list of pore nodes (pore-list) [6,18].

The current paper focuses on a detailed comparison of some of these possible implementation details to accurately estimate the permeability of porous media with the LB method. We compare the well known D3Q19 single relaxation (LB-BGK) [5,19] and multirelaxation time (LB-MRT) [2,20] models together with three alternative setups to estimate the permeability utilizing an injection channel (I-Ch), pressure boundary conditions (p-BC), or a sample force density (∇p-$\mathcal{S}$). The geometries being investigated are a 3D Poiseuille flow in a square pipe and a *BCC* sphere array. While the first one has the advantage of a minimal discretization error, the second one more realistically resembles a natural porous medium. We also present a comparison of the efficiency of the LB-codes based on the above mentioned pore-matrix and pore-list data structures [18].

2 The Lattice-Boltzmann method

The discretized lattice-Boltzmann (LB) equation reads

$$n_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - n_i(\mathbf{x},t) = \Delta t \sum_{j=1}^{N} S_{ij}\Big(n_j(\mathbf{x},t) - n_j^{\mathrm{eq}}(\mathbf{x},t)\Big), \tag{2.1}$$

where $\mathbf{x}=(x_1,x_2,x_3)$ represents a node. The discretization parameters are Δt and Δx, while the discrete velocities $\mathbf{c}_i$ have the dimension $\Delta x/\Delta t$. The variable n_i is the probable number of particles moving with velocity $\mathbf{c}_i$. We use a 3D cubic lattice with 19 discrete velocities $\mathbf{c}_i$, $i=1\cdots,19$, known as D3Q19 (see Fig. 1 for a visualization) [4]. The term on the right hand side of Eq. (2.1) is the linearized collision operator, where S_{ij} is the collision matrix also known as scattering matrix and $n_j^{\mathrm{eq}}(\mathbf{x},t)$ is the equilibrium distribution [2]. The macroscopic density $\rho(\mathbf{x},t)$ and velocity $\mathbf{u}(\mathbf{x},t)$ are obtained