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Coarse- and fine-grid numerical behavior of MRT/TRT lattice-Boltzmann schemes in regular and random sphere packings

Siarhei Khirevich [a], Irina Ginzburg [b,*], Ulrich Tallarek [a]

[a] Department of Chemistry, Philipps-Universität Marburg, Hans-Meerwein-Strasse, 35032 Marburg, Germany
[b] Irstea, Antony Regional Centre, HBAN, 1 rue Pierre-Gilles de Gennes CS 10030, 92761 Antony Cedex, France

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ABSTRACT

We analyze the intrinsic impact of free-tunable combinations of the relaxation rates controlling viscosity-independent accuracy of the multiple-relaxation-times (MRT) lattice-Boltzmann models. Preserving all MRT degrees of freedom, we formulate the parametrization conditions which enable the MRT schemes to provide viscosity-independent truncation errors for steady state solutions, and support them with the second- and third-order accurate ("linear" and "parabolic", respectively) boundary schemes. The parabolic schemes demonstrate the advanced accuracy with weak dependency on the relaxation rates, as confirmed by the simulations with the D3Q15 model in three regular arrays (SC, BCC, FCC) of touching spheres. Yet, the low-order, bounce-back boundary rule remains appealing for pore-scale simulations where the precise distance to the boundaries is undetermined. However, the effective accuracy of the bounce-back crucially depends on the free-tunable combinations of the relaxation rates. We find that the combinations of the kinematic viscosity rate with the available "ghost" antisymmetric collision mode rates mainly impact the accuracy of the bounce-back scheme. As the first step, we reduce them to the one combination (presented by so-called "magic" parameter Λ in the frame of the two-relaxation-times (TRT) model), and study its impact on the accuracy of the drag force/permeability computations with the D3Q19 velocity set in two different, dense, random packings of 8000 spheres each. We also run the simulations in the regular (BCC and FCC) packings of the same porosity for the broad range of the discretization resolutions, ranging from 5 to 750 lattice nodes per sphere diameter. A special attention is given to the discretization procedure resulting in significantly reduced scatter of the data obtained at low resolutions. The results reveal the identical Λ-dependency versus the discretization resolution in all four packings, regular and random. While very small Λ values overestimate the drag measurements several-fold on the coarse grids, $\Lambda > 1$ may overestimate the permeability at the same extent. In low resolution region we provide practical guidelines, extending previously known solutions for the straight/diagonal Poiseuille flow. Analysis of the high-resolution region reveals the collapse of the solutions obtained with all the considered Λ values with the average rate of -1.3, followed by their common, smooth, first-order convergence with the rate of -1.0 as the best, towards the reference solutions provided by the "parabolic" schemes. High-quality power-law fits

* Corresponding author.
E-mail addresses: khirevich@gmail.com (S. Khirevich), irina.ginzburg@irstea.fr (I. Ginzburg), tallarek@staff.uni-marburg.de (U. Tallarek).

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estimate that the bounce-back would reach their accuracy (obtained at about 200 nodes per sphere) for two-order magnitude higher grid resolution.

1. Introduction

Modeling Stokes and moderate Reynolds number flows has received a particular attention in analysis [11,16,18,35,36,74] and benchmarking [7,8,14,15,38,52,57,62,67] of the Lattice Boltzmann Method (LBM). The method, pioneered in early works [47,48,65] (see also references in [35]), is appealing for the simulations of flow in reconstructed porous media [3,5,31,45,58–60,71,72] as well as of complex fluids [2,49]. An easiness of the LBM simulations at a pore scale is mainly due to the bounce-back rule which mimics the no-slip boundary condition with no need either for re-meshing near the complex solid obstacles or for computing the distance to them. However, the flipside of this simplicity is the well recognized numerical artefact, an eventual dependency of the effective (modeled) pore size upon the viscosity of the simulated fluid. Although this problem has been explored analytically [18,35] and the remedy was found in using the two-relaxation-time (TRT) collision configuration [20,22], in this work we return to it because of the following issues:

- Over the last decade full multiple-relaxation-times (MRT) configurations [34] became popular for the simulations of laminar flow. The MRT model matches the TRT when one relaxation parameter is chosen for all symmetric and another — for all anti-symmetric modes; the specific combinations of the relaxation parameters should remain fixed when the transport coefficient varies. However, configurations [34] of the relaxation parameters optimized for stability in non-linear flow, or those configurations where only kinematic and bulk viscosity vary for the fixed rate of all "ghost" modes [1,8,30] do not provide viscosity-independent permeability results, which can explain deficiency observed in studies [59,60,67]. In this work we will address the proper selection of the MRT relaxation parameters without reducing MRT to TRT, and illustrate impact of the most important "ghost" modes by simple analytical and numerical examples.
- The bounce-back rule together with the proper set of the relaxation rates keeps permeability viscosity-independent, but the permeability is still affected by all free-tunable relaxation combinations assigned for symmetric and anti-symmetric modes. Thereby, we analyze the impact of those combinations on the velocity field simulated in complex geometries, and discuss their proper selection. Our analysis is based on the detailed study of the drag force simulated in two random packings of 8000 spheres each and two regular (BCC and FCC) packings. This study covers a broad range of the discretization resolutions, from very coarse (4 nodes per sphere diameter) to very fine (750 nodes), enabling observation of the asymptotic behavior.
- Accuracy of the bounce-back can be improved via the "linear" schemes [6,8,22,23], but the aforementioned dependency on the free relaxation rates becomes insignificant only for the "parabolic" schemes [18,22,23]. Previously developed and parametrized in the TRT setup, in this work we extend these schemes for the MRT collision operator. We demonstrate that the "parabolic" schemes produce velocity fields of the reference quality on relatively coarse grids, and examine the convergence of the bounce-back to their solutions. We also make "linear" schemes [6] able to produce viscosity-independent permeability results by the means of proper corrections.

In this work we consider modeling the stationary Stokes equation describing flow of an incompressible fluid of the kinematic viscosity ν:

$$\nabla P - \vec{F} = \nu \Delta \vec{j}, \tag{1a}$$

$$\nabla \cdot \vec{j} = 0, \tag{1b}$$

$$\vec{j} = \rho_0 \vec{u}. \tag{1c}$$

The effective conductivity of d-dimensional geometric structure can be quantified via its (symmetric) permeability tensor $\mathbf{K}[d \times d]$, which relates via Darcy's law the superficial mass flux $\varepsilon \bar{\vec{j}}$ in porous sample of porosity ε to the applied driving force $\overline{\vec{F} - \nabla P}$:

$$\varepsilon \bar{\vec{j}} = \frac{\mathbf{K}}{\nu} \overline{\vec{F} - \nabla P}. \tag{2}$$

For Newtonian fluids the permeability does not depend on the kinematic viscosity, and therefore Darcy's number (or non-dimensional permeability, k/L^2) quantifies the Stokes flow in the following sense: giving the `fluid`/`solid` geometry and the driving force $\overline{\vec{F} - \nabla P}$, the solution of (2) has to remain the same for $\nu \bar{\vec{j}}$ when ν varies. In other words, the numerical method for solving the Stokes equation should maintain its linearity exactly. However, the obtained Darcy's number may depend on the spatial resolution due to the discretization effects, unless the numerical scheme reaches its asymptotic limit.