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An improved gray lattice Boltzmann model for simulating fluid flow in multi-scale porous media

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ABSTRACT

A lattice Boltzmann (LB) model is proposed for simulating fluid flow in porous media by allowing the aggregates of finer-scale pores and solids to be treated as 'equivalent media'. This model employs a partially bouncing-back scheme to mimic the resistance of each aggregate, represented as a gray node in the model, to the fluid flow. Like several other lattice Boltzmann models that take the same approach, which are collectively referred to as gray lattice Boltzmann (GLB) models in this paper, it introduces an extra model parameter, n_s, which represents a volume fraction of fluid particles to be bounced back by the solid phase rather than the volume fraction of the solid phase at each gray node. The proposed model is shown to conserve the mass even for heterogeneous media, while this model and that model of Walsh et al. (2009) [1], referred to the WBS model thereafter, are shown analytically to recover Darcy–Brinkman's equations for homogenous and isotropic porous media where the effective viscosity and the permeability are related to n_s and the relaxation parameter of LB model. The key differences between these two models along with others are analyzed while their implications are highlighted. An attempt is made to rectify the misconception about the model parameter n_s being the volume fraction of the solid phase. Both models are then numerically verified against the analytical solutions for a set of homogenous porous models and compared each other for another two sets of heterogeneous porous models of practical importance. It is shown that the proposed model allows true no-slip boundary conditions to be incorporated with a significant effect on reducing errors that would otherwise heavily skew flow fields near solid walls. The proposed model is shown to be numerically more stable than the WBS model at solid walls and interfaces between two porous media. The causes to the instability in the latter case are examined. The link between these two GLB models and a generalized Navier–Stokes model [2] for heterogeneous but isotropic porous media are explored qualitatively. A procedure for estimating model parameter n_s is proposed.
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1. Introduction

Lattice Boltzmann (LB) method [3–7] has proven to be a promising mesoscale method and been widely used to simulate physical behaviors of fluid flow and solute transport for engineering applications for the past two decades. Thanks to advances in high-resolution imaging, LB has been gaining greater popularity in many disciplines of science and engineering in which the fluid flow and solute transport behaviors in porous media are of concern [8–10]. LB is known to be superior to many classical Computational Fluid Dynamics (CFD) methods due to its computational simplicity, its amenability to simple and efficient implementation and parallelization, and its ability of handling geometrically complex porous media. Despite all of these, it remains to be very challenging and costly to perform LB flow simulation in porous media. This is because any useful porous model must represent a large sample and be able to resolve pores of various sizes from its image (e.g. by 3D X-ray CT imaging) explicitly into fluid and solid nodes to produce a binary characterization of its pore system. Such a characterization can only be done accurately when pores and solid materials are well resolved by imaging instruments and when image pixel/voxel values can be well calibrated against the imaged samples. For natural porous media like soils and sedimentary rocks, which are spatially heterogeneous at many different scales, both in terms of the material compositions and pore structure, neither of the two conditions is likely to be met satisfactorily for some of pixels/voxels. Those pixels/voxels are therefore gray-ish in the sense that they may represent the aggregates of pores and solids at smaller scales than the resolution of the imaging instrument. However, their grayness may indeed correlate with sub-resolution pore structures [11]. If they are to be binarised or segmented, some subjective or semi-objective criteria need be applied, and this may lead to inaccurate binary outcomes. A study by Baveye et al. [12] highlights the magnitude of this problem in an experiment where three 2D images of soil samples are given to a group of specialists and fed to several

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computer-automated segmentation procedures to produce binary images. The authors show that for each sample image a large variability is observed among the outcomes binarised by the specialists and it is even larger among those by the computer-automated procedures. It has been shown (see [13]) that a better binary characterization may be achieved by constraining the binarization on some measurements of a sample, e.g. porosity. However, this approach is still insufficient to treat the subscale pores and solids and therefore in effect ignores subscale information. It is well known that fluid flow and solute transport behaviors within sub-micron pores are of particular importance in many applications, including pollution remediation in soils, hydrocarbon production from carbonate rocks, and CO2 storage at the subsurface.

Models of the subscale pores and solids may be constructed by higher-resolution 2/3D imaging on samples of much smaller sizes in conjunctions with stochastic modeling [14,15]. If multi-scale models are to be stitched together into a single binary model, that model is likely to contain too many pore nodes, rendering standard LB simulations inefficient and even intractable even with newly-developed LB simulation schemes (Refs: [9,16–21]), because it would require excessive computer resources to operate. Therefore, LB models that are capable of treating the gray-ish pixels/voxels as equivalent media in flow simulations become appealing.

A number of LB models have been developed to allow each lattice node to be either fluid, solid or gray node, where a gray node represents an aggregate of finer scale pores and solids as ‘equivalent media’. A key issue in developing these models is to model the resistance of each aggregate to the fluid flow correctly. This is often done by two approaches. The first approach accounts for the flow resistance in the standard LB models by modifying body-force or equilibrium terms, leading to the recovery of either Darcy–Brinkman’s equations or generalized Navier–Stokes equations [2,16,22,23]. Although this approach has been applied for modeling fluid flow at a regional scale [24], it has been pointed out by the authors in [25,26] that the Chapman–Enskog expansion for deriving the corresponding macroscopic equations may break down. Unlike the first approach, the second one introduces a partial bounce-back term on fluid particles at each gray node, prior to LB streaming operation. A correct partial bounce-back term of a model mimics the resistance of each porous aggregate to fluid flow. LB models developed using this approach are referred to as Gray Lattice Boltzmann (GLB) models, and are of concern in this paper.

In the second approach, the partial-bounceback term may simply take a form of $n_s\delta f$, where n_s is a model parameter, representing a volume fraction of net fluid particles, δf, to be bounced back due to the existence of solid phase. Four GLB models, which have been proposed in [27–29] and [1], respectively, take the same form of the partial-bounceback term, and are labeled as GS, DMC, TS, and WBS, respectively, for later use. As it has been (see [30,1]) and will be further shown later in this paper for the WBS model and a model to be proposed, the partial-bounceback term $n_s\delta f$ leads to the Darcy term too, and therefore, the GLB models are equivalent to those “body-force term” models of the first approach.

In each GLB model, the term $n_s\delta f$ must be specified so that (1) the mass is conserved even for heterogeneous porous media; (2) the underlying porous medium specified by n_s is in consistence with flow resistance that the partial-bounceback simulates. Walsh et al. [1] showed that several GLB models mentioned above do not conserve the mass for heterogeneous porous media. The second criterion is a pre-requirement to apply any GLB model, but more difficult to meet. Natural porous media are intricately heterogeneous in terms of pore structure and the composition of the solid phases, and both the pore structure and the solid composition control the fluid flow behavior of a given fluid. There have been attempts to relate n_s, rather superficially, to a volume fraction of the solid phase in the previous work. Walsh et al. [1] realized this to be indeed inappropriate not only for setting up a simulation but also for interpreting the results. However, they failed to rectify this misconception fully in their work but kept using inappropriate terminology - a volume fraction of the solid phase instead. Indeed, they assume a mapping between the permeability and n_s can be determined via the actual volume fraction of the solid phase alone. They did not realize that n_s is related to the fluid viscosity too. In practical work, n_s may be estimated using information on the pore structure and the solid composition (e.g. gray-scale X-ray CT images) to be calibrated with laboratory flow measurement for a given fluid. A procedure is proposed in this work.

The main contributions of this paper are as follows. It presents a new GLB model that meets the two criteria above. Unlike other GLB models, the partial-bounceback term of the proposed model is constructed based on a natural repartition of fluid particles before being streamed, where n_s defines precisely and unambiguously the volume fraction of fluid particles to be bounced back at each gray node. It proves that both the proposed model and the WBS model recover the Darcy–Brickman flow under an ideal flow condition with the derivations of effective viscosity and permeability for both models. It analyses both models along with others, offering a better understanding of their macro-scale flow behaviors. The proposed and WBS models are verified against analytical solutions and numerically compared for simple but practically meaningful porous models. These comparisons reveal the proposed model to be superior in numerical stability and handling no-slip boundary conditions at solid walls. Both models are shown to be equivalent to a LB model with an extended force term for solving generalized Navier–Stokes equations [2]. To make GLB models for practical uses, a procedure for determining n_s is proposed.

This paper is organized as follows. Section 2 gives a brief introduction to LB notations used in this paper and existing GLB models before proposing a new model. Section 3 analyzes the proposed model and the WBS model, which has not been analyzed previously for the latter, and shows that both models recover the Darcy–Brickman flow with respective effective viscosity but the identical permeability, up to a transformation of n_s. The derivations are given in, Appendix A.1. Section 4 shows numerical verification of the proposed and WBS models and numerical comparisons for three types of porous models. In Section 5, remarks and discussions are made on the link of the two GLB models and a LB model with an extended force term, the drawbacks of the WBS model in numerical stability, and an approach to estimate n_s for practical use followed by a conclusion.

2. Existing GLB and a new GLB model

Prior to the main discussion of this section, some basics of the LB method are given below to introduce the notations to be used later.

Let $f(\xi,\mathbf{r},t)$ denote particle distribution function (PDF), meaning the probability of finding a fluid particle with a velocity ξ at location $\boldsymbol{r}$ and time t. The Boltzmann-BGK equation reads [31]

$$\frac{\partial f(\xi,\mathbf{r},t)}{\partial t}+\xi\cdot\frac{\partial f(\xi,\mathbf{r},t)}{\partial \mathbf{r}}+\frac{1}{\rho}\mathbf{F}\cdot\frac{\partial f(\xi,\mathbf{r},t)}{\partial \xi}=-\frac{f-f^{eq}}{\tau} \tag{1}$$

where $\mathbf{F}$, $\rho=\rho(\mathbf{r},t)$ and f^{eq} are the force acting on the unit volume, the mass density, and an equilibrium distribution function, respectively. On a standard lattice of the form DdQb [7] with directions $\mathbf{e}_\alpha$ where $\alpha=1,2,\ldots b$, let $\xi_\alpha=\frac{\Delta x}{\Delta t}\mathbf{e}_\alpha$ be the corresponding discrete velocity where Δx is the length of a lattice cell and Δt is the time step, and $f_\alpha=f_\alpha(\mathbf{r},t)\equiv mf(\xi_\alpha,\mathbf{r},t)$ – the discrete PDF, and define the dimensionless variables as shown in Table 1. Symbols in that table will be used exclusively in what it follows.

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