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Two-relaxation-time lattice Boltzmann method and its application to advective-diffusive-reactive transport

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ABSTRACT

The lattice Boltzmann method (LBM) based on single-relaxation-time (SRT) or multiple-relaxation-time (MRT) collision operators is widely used in simulating flow and transport phenomena. The LBM based on two-relaxation-time (TRT) collision operators possesses strengths from the SRT and MRT LBMs, such as its simple implementation and good numerical stability, although tedious mathematical derivations and presentations of the TRT LBM hinder its application to a broad range of flow and transport phenomena. This paper describes the TRT LBM clearly and provides a pseudocode for easy implementation. Various transport phenomena were simulated using the TRT LBM to illustrate its applications in subsurface environments. These phenomena include advection-diffusion in uniform flow, Taylor dispersion in a pipe, solute transport in a packed column, reactive transport in uniform flow, and bacterial chemotaxis in porous media. The TRT LBM demonstrated good numerical performance in terms of accuracy and stability in predicting these transport phenomena. Therefore, the TRT LBM is a powerful tool to simulate various geophysical and biogeochemical processes in subsurface environments.

1. Introduction

Important biogeochemical processes such as microbial metabolism and contaminant remediation take place at the pore scale in subsurface environments (Meakin and Tartakovsky, 2009; Nambi et al., 2003; Wang and Long, 2012; Yan et al., 2016). Pore-scale modeling allows to directly examine the biogeochemical processes and is able to provide mechanistic insights into macroscopic field observations (Blunt et al., 2013; Yoon et al., 2015). The Lattice Boltzmann method (LBM) is one of the most widely used pore-scale methods (Aidun and Clausen, 2010; Chen and Doolen, 1998; Liu et al., 2016; Long and Hilpert, 2008), and has been used to study various geophysical and biogeochemical processes in porous and fractured media, including solute transport (Calì et al., 1992), contaminant remediation (Parales et al., 2000; Yan et al., 2014), geologic carbon storage (Kang et al., 2010; Tian et al., 2014), and mineral cementation and dissolution (Chen et al., 2014; Kang et al., 2003; 2002). Recently, the LBM has been used to tackle more challenging problems such as heat transfer in thermofluids (Li et al., 2016b) and complex flow and reactions in nanoporous catalysts (Falcucci et al., 2017; 2016; Montessori et al., 2015; 2016).

The LBM captures the physics of macroscopic behaviors through controlling the local mesoscopic operations of pseudo-particles that move on a regular lattice, with a set of discrete velocities, and relax to an equilibrium state via a collision operator (Aidun and Clausen, 2010; Benzi et al., 1992; Chen and Doolen, 1998; Guo and Shu, 2013; Higuera et al., 1989). The distribution and evolution of the particles determine how the solute concentration changes with respect to space and time. The typically explicit, numerical time-stepping scheme makes it easy to develop a LBM code (Succi, 2001), and the local nature of the LBM makes it suitable for parallel computing (Groen et al., 2013). Moreover, the LBM is well suited to deal with potentially reactive surface boundaries in complex pore geometries through using simple or modified bounce-back schemes (Chen et al., 2015; He et al., 1997; Kang et al., 2006; Pan et al., 2006). These characteristics enable the LBM to explore a variety of flow and transport phenomena in complicated geometries (Aidun and Clausen, 2010; Yoon et al., 2015).

Different selections of the collision operator result in three typical LBMs: single-relaxation-time (SRT) LBM, two-relaxation-time (TRT) LBM, and multiple-relaxation-time (MRT) LBM. These LBMs are different in terms of numerical accuracy and stability (Luo et al., 2011). The SRT LBM employs a single relaxation parameter and is easy to implement (Chen and Doolen, 1998). It is the most popular LBM but may suffer from unphysical artifacts in

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complicated geometries and numerical instability at small relaxation rates (He et al., 1997; Luo et al., 2011). The MRT LBM employs multiple relaxation parameters, and can attain more stable and accurate simulations by tuning the relaxation parameters (Yan and Hilpert, 2014). However, selecting the multiple relaxation parameters is challenging since it requires comprehensive asymptotic analysis (d'Humières et al., 2002; Yan and Hilpert, 2014). The TRT LBM employs two relaxation parameters to relax the particle distributions, having one fixed but the other tunable (Ginzburg, 2005a; 2005b). It maintains the simplicity of the SRT method in terms of implementation while retaining the advantages of the MRT method in terms of numerical accuracy and stability (Luo et al., 2011).

Since its systematic development the TRT LBM has been applied to both flow and transport phenomena (Ginzburg, 2005a), such as permeability estimation in different geometries (Talon et al., 2012), multi-phase flow in porous media (Genty and Pot, 2013; Liu et al., 2014), advection-diffusion in bulk flow (Servan-Camas and Tsai, 2008), and effective diffusion in unsaturated porous media (Genty and Pot, 2014). However, the TRT LBM is rarely used in reactive transport, which is of great significance for many biogeochemical processes in subsurface environments (Li et al., 2016a). The TRT method is also much less used than the SRT and MRT LBMs, although it integrates the simplicity of the SRT method and the stability of the MRT method. One reason is that the tedious mathematical derivations and presentations of the TRT method hinder its understanding and implementation (Ginzburg, 2005a; 2012; Ginzburg et al., 2010; 2008). Therefore, a clear presentation of the TRT LBM is necessary for extending its applications to a broader variety of flow and transport phenomena.

This paper aims to articulate the framework and implementation of the TRT LBM as simply as possible and to apply this method to various transport phenomena. We provide a clear description of the TRT LBM including a pseudocode for straightforward implementation. The method was applied to a variety of transport phenomena to demonstrate its ability to reproduce subsurface phenomena. Advective-diffusive-reactive transport in uniform flow, for which analytical solutions are available, was examined to evaluate the stability and accuracy of the TRT method used in simple geometries. Taylor dispersion in a pipe was examined to assess the effect of solid boundaries on the stability and accuracy. Solute transport in a packed column was examined to assess the numerical performance of the TRT method in complicated geometries. Lastly, bacterial chemotaxis in porous media was examined to illustrate the application of the TRT method to biogeochemical reactions in subsurface environments.

2. Methods

The thermodynamic state of a solute in the TRT LBM is defined by a Q-dimensional particle distribution function, $f_q(\mathbf{r}, t)$, where $q = 0, \ldots, Q-1$. This function is defined at each lattice node ($\mathbf{r}$) and for each discrete time (t). The nodes in the lattice space are connected by a set of discrete velocities $\mathbf{c}_q$ which are aligned with lattice axes and diagonals. Summing up the particle distributions over all the discrete velocities yields the solute concentration C:

$$C = \sum_{q=0}^{Q-1} f_q \tag{1}$$

At each node, the particle distribution function can be decomposed into symmetric and antisymmetric components,

$$f_q = f_q^+ + f_q^- \tag{2}$$

where $f_q^+ = (f_q + f_{\bar{q}})/2$ and $f_q^- = (f_q - f_{\bar{q}})/2$. The integer $\bar{q}$ is the index of velocity $\mathbf{c}_{\bar{q}}$ that points to the opposite direction of $\mathbf{c}_q$ ($\mathbf{c}_{\bar{q}} = -\mathbf{c}_q$). For the rest of the particles that have a zero velocity ($\mathbf{c}_0 = 0$), $f_0^+ = f_0 = C - \sum_{q=1}^{Q-1} f_q$ and $f_0^- = 0$. In order to simplify the sums over all velocities $\mathbf{c}_q$, we assume that the velocities are ordered such that $\bar{q} = q + (Q-1)/2$ for $1 \le q \le (Q-1)/2$. Therefore $f_0^+ = C - 2\sum_{q=1}^{(Q-1)/2} f_q^+$.

The particles at one node move to neighboring nodes in terms of the non-zero discrete velocities $\mathbf{c}_q$ ($\mathbf{c}_q \neq 0$, $q = 1, \ldots, Q-1$), or stay at the node for $\mathbf{c}_0$. Once the particles reach the neighboring nodes, the resultant distributions are relaxed to an equilibrium state through a TRT collision operator (Ginzburg, 2005a):

$$f_q(\mathbf{r} + \mathbf{c}_q, t+1) = \underbrace{f_q(\mathbf{r}, t) - \frac{1}{\tau^+}(f_q^+ - e_q^+) - \frac{1}{\tau^-}(f_q^- - e_q^-)}_{\tilde{f}_q(\mathbf{r}, t)} \tag{3}$$

where e_q^+ and e_q^- are the symmetric and antisymmetric components of the equilibrium particle distribution e_q ($e_q = e_q^+ + e_q^-$); τ^+ and τ^- are the symmetric and antisymmetric relaxation parameters, respectively. The entire right hand side of Eq. (3) is called post-collision particle distribution $\tilde{f}_q(\mathbf{r}, t)$.

The equilibrium particle distributions for a non-zero discrete velocity can be expressed by (Ginzburg, 2013)

$$e_q^+ = C\left(t_q^{(m)} c_s^2 + t_q^{(u)}\overline{V^2} + w_q^{(u)}\|\mathbf{c}_q\|^2 \sum_{\alpha=1}^{d}(V_\alpha^2 - \overline{V^2})c_{q\alpha}^2 + \sum_{\beta\neq\alpha} \frac{V_\alpha V_\beta c_{q\alpha} c_{q\beta}}{2\sum_{j=1}^{(Q-1)/2} c_{j\alpha}^2 c_{j\beta}^2}\right) \tag{4}$$

and

$$e_q^- = t_q^{(a)} C \sum_{\alpha=1}^{d} V_\alpha c_{q\alpha} \tag{5}$$

where $q = 1, \ldots, (Q-1)/2$, V_α (or V_β) are the αth (or βth) Cartesian component of the advective velocity in the lattice space, $\overline{V^2} = \sum_{\alpha=1}^{d} V_\alpha^2/d$ where d is the dimensionality (i.e., $d = 3$ for a three-dimensional LBM), $c_{q\alpha}$ is the αth Cartesian component of the discrete velocity $\mathbf{c}_q$, c_s is the speed of sound, $t_q^{(m)}$, $t_q^{(u)}$, $w_q^{(u)}$ and $t_q^{(a)}$ are weights. All these weights are non-negative and isotropic, and satisfy the isotropy conditions:

$$\sum_q w_q^{(\cdot)} c_{q\alpha} c_{q\beta} = \delta_{\alpha\beta}, \quad \sum_q t_q^{(\cdot)} c_{q\alpha} c_{q\beta} = \delta_{\alpha\beta} \tag{6}$$

where $\alpha, \beta = 1, \ldots, d$. Different selections of the weights result in different numerical stabilities (Ginzburg et al., 2010).

The other half of the equilibrium particle distributions (for $q = (Q-1)/2+1, \ldots, Q-1$) can be calculated through the symmetric and antisymmetric relations

$$e_{\bar{q}}^+ = e_q^+ \quad \text{and} \quad e_{\bar{q}}^- = -e_q^- \tag{7}$$

For the rest of the particles, $e_0^+ = C - 2\sum_{q=1}^{(Q-1)/2} e_q^+$ and $e_0^- = 0$.

To make the TRT method as simple as possible, we apply the widely used standard bounce-back (SBB) boundary condition:

$$f_{\bar{q}}(\mathbf{r}, t+1) = \tilde{f}_q(\mathbf{r}, t), \tag{8}$$

which mimics the phenomenon that a particle is reflected back into the pore domain when colliding with a solid boundary.

If there exists mass source or sink (M), the post-collision particle distributions are modified to:

$$\begin{aligned} \tilde{f}_q(\mathbf{r}, t) &= \tilde{f}_q(\mathbf{r}, t) + t_q^{(m)} c_s^2 M, \quad q = 1, \ldots, Q-1 \\ \tilde{f}_0(\mathbf{r}, t) &= \tilde{f}_0(\mathbf{r}, t) + M\left(1 - 2c_s^2 \sum_{q=1}^{(Q-1)/2} t_q^{(m)}\right) \end{aligned} \tag{9}$$

where $\tilde{f}_q$ on the right-hand-sides is defined in Eq. (3). This modification enables the TRT LBM to simulate reactive transport.