Commun. Comput. Phys.
doi: 10.4208/cicp.181015.270416a

Vol. **20**, No. 2, pp. 374-404
August 2016

Do Current Lattice Boltzmann Methods for Diffusion and Advection-Diffusion Equations Respect Maximum Principle and the Non-Negative Constraint?

S. Karimi and K. B. Nakshatrala*

Department of Civil and Environmental Engineering, University of Houston, USA.

Received 18 October 2015; Accepted (in revised version) 27 April 2016

Abstract. The Lattice Boltzmann Method (LBM) has established itself as a popular numerical method in computational fluid dynamics. Several advancements have been recently made in LBM, which include multiple-relaxation-time LBM to simulate anisotropic advection-diffusion processes. Because of the importance of LBM simulations for transport problems in subsurface and reactive flows, one needs to study the accuracy and structure preserving properties of numerical solutions under the LBM. The solutions to advective-diffusive systems are known to satisfy maximum principles, comparison principles, the non-negative constraint, and the decay property. In this paper, using several numerical experiments, it will be shown that current single- and multiple-relaxation-time lattice Boltzmann methods *fail* to preserve these mathematical properties for transient diffusion-type equations. We will also show that these violations may not be removed by simply refining the discretization parameters. More importantly, it will be shown that meeting stability conditions alone does not guarantee the preservation of the aforementioned mathematical principles and physical constraints in the discrete setting. A discussion on the source of these violations and possible approaches to avoid them is included. A condition to guarantee the non-negativity of concentration under LBM in the case of isotropic diffusion is also derived. The impact of this research is twofold. *First*, the study poses several outstanding research problems, which should guide researchers to develop LBM-based formulations for transport problems that respect important mathematical properties and physical constraints in the discrete setting. This paper can also serve as a good source of benchmark problems for such future research endeavors. *Second*, this study cautions the practitioners of the LBM for transport problems with the associated numerical deficiencies of the LBM, and provides guidelines for performing predictive simulations of advective-diffusive processes using the LBM.

AMS subject classifications: 65-XX

Key words: Lattice Boltzmann method (LBM), meso-scale modeling, multiple-relaxation-time, advection-diffusion equations, comparison principle, maximum principle, non-negative constraint, anisotropy, statistical mechanics.

*Corresponding author. *Email address:* knakshatrala@uh.edu (K. B. Nakshatrala)

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1 Introduction and motivation

The lattice Boltzmann method (LBM) has gained remarkable popularity as a versatile numerical method for fluid dynamics simulations [12]. LBM has its roots in the kinetic theory as opposed to the continuum theory. It needs to be emphasized that LBM solves the Boltzmann equation instead of solving the continuum field equations. On the other hand, the finite element method (FEM) and the finite volume method (FVM) solve the continuum field equations directly. The lattice Boltzmann method has many attractive features, for instance: (1) It can easily handle irregular domains (e.g., unstructured pores and fractures in porous media applications), (2) It is easy to implement even for complicated flow models, (3) It is natural to parallelize even in a heterogeneous computing setup [43]. Some recent advances are extension of LBM to simulate multi-phase flows [20], reactive flows [35], non-linear chemical reactions [2], just to name a few.

Advection-diffusion equation plays a vital role in modeling a variety of physical phenomena. For instance, modeling of reactive-transport [7, 41], simulation of drug delivery in blood [36, 39], transport of chemical species in porous media [4, 29]. Consequently, extension of the LBM to advection-diffusion equation has been the focus of major scientific research. In recent years, several key advancements have been made to extend the LBM to simulate transport phenomena. To name a few: [9, 23, 38, 42, 46]. Of these works, Yoshida and Nagaoka [46], and Huang and Wu [23] have proposed multiple-relaxation-time lattice Boltzmann methods to solve advection-diffusion equations with *anisotropic* diffusivity tensors. However, a numerical method can never be considered attractive for predictive simulations, unless it preserves some (if not all) of the mathematical properties of the equations it is aiming to solve.

The governing equations for transient advective-diffusive systems are parabolic partial differential equations, which possess several important mathematical properties. These properties include the maximum principle and the comparison principle [33, 34], which have crucial implications in modeling physical phenomena. For example, a key consequence of the maximum principle in modeling advective-diffusive systems is the non-negative constraint of the attendant chemical species. Violations of these mathematical properties can make a numerical solution inappropriate for scientific and engineering applications.

It has been shown that many popular finite element and finite volume formulations for diffusion-type equations violate the maximum principle and the non-negative constraint [27,30,32]. Several factors such as the physical properties of the medium, topology of the domain, and the spatial and temporal discretization determine the performance of a numerical solution in preserving the *discrete* versions of the aforementioned mathematical properties. A discussion on the influence of these factors in the context of the finite element method can be found in [30]. Note that a numerical method can be shown to "converge" to the exact solution, but it may not always preserve the mentioned properties. Recently, numerical methodologies have been proposed under the finite element method to satisfy the non-negative constraint and the maximum principle by utilizing