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A Lattice Boltzmann Method for the Advection-Diffusion Equation with Neumann Boundary Conditions

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Abstract. In this paper, we study a lattice Boltzmann method for the advection-diffusion equation with Neumann boundary conditions on general boundaries. A novel mass conservative scheme is introduced for implementing such boundary conditions, and is analyzed both theoretically and numerically.

Second order convergence is predicted by the theoretical analysis, and numerical investigations show that the convergence is at or close to the predicted rate. The numerical investigations include time-dependent problems and a steady-state diffusion problem for computation of effective diffusion coefficients.

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1 Introduction

The lattice Boltzmann method (LBM) has received much attention for flow simulation since its introduction in the 1990's [2,4,9]. Although much less discussed, it is well known that the LBM can be applied to diffusion and advection-diffusion equations as well, see e.g. [7,13,14,16]. Applications include solute transport in porous media [13], dissolution phenomena [17], dispersion [18,19] and comparisons to NMR experiments [10].

To be precise, the problem we study in this paper is the advection-diffusion equation with isotropic diffusion

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{U})=D\Delta\rho \quad \text{in } \Omega\times[0,T], \tag{1.1a}$$

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$$\rho|_{t=0}=\rho_0 \quad \text{in } \Omega, \tag{1.1b}$$

$$\partial_n \rho = 0 \qquad \text{on } \partial\Omega\times[0,T], \tag{1.1c}$$

where ρ is the density, $\mathbf{U}$ is a given flow velocity and D is a scalar diffusion coefficient. All the analysis will be valid for this equation, although for the numerical results, we will set $\mathbf{U}=0$, which yields the isotropic diffusion equation with Neumann (zero normal flux) boundary conditions.

When applying the lattice Boltzmann method, macroscopic variables such as ρ in (1.1) are obtained as moments in velocity space of a distribution function f. The evolution of f is described by the lattice Boltzmann equation (LBE)

$$f_i(t+\Delta t,\mathbf{x}+\mathbf{c}_i\Delta t)-f_i(t,\mathbf{x})=J_i(f,f^{(eq)}), \qquad i=0,\cdots,q-1, \tag{1.2}$$

where q is the number of discrete velocities used, $\{\mathbf{c_i}\}_{i=0}^{q-1}$ is the set of velocities, and $J_i(f,f^{(eq)})$, $i=0,\cdots,q-1$ are collision operators describing the relaxation of f towards an equilibrium distribution $f^{(eq)}$. The LBM is applied using a time-splitting approach, first applying a collision step to compute the right hand side of (1.2) and then a streaming step to move the distribution according the velocities $\mathbf{c}_i$, as prescribed by the left hand side of (1.2).

The way boundary conditions in the lattice Boltzmann method are applied is slightly different compared to other numerical methods. Since the LBM simulates the time evolution of a velocity distribution, and macroscopic quantities like density are only obtained as moments of this distribution, boundary conditions have to determine the whole particle distribution, and not only the density or flux that is determined by the macroscopic boundary condition (such as a Dirichlet or Neumann boundary condition). This has to be done in a consistent way in order not to reduce accuracy and/or stability for the solution to the macroscopic equation.

Neumann and other flux boundary conditions for the diffusion equation have not been much studied in the LBM framework, despite the fact that they present certain challenges, as will be seen below. In some cases [11], the bounce-back boundary condition has been applied, which is erroneous as it prescribes not only zero normal flux, but also zero tangential flux. In other cases [13, 17], the Neumann boundary condition has been correctly applied, but only for grid-aligned boundaries, where it is rather easily implemented through specular reflection of the velocity distribution, see [7].

For general boundaries, we have found only two attempts at a proper implementation of flux boundary conditions. Yoshida et al. [18] introduced corrections to the bounce-back rule in order to get a correct total flux through a surface, when the (non-zero) flux was prescribed at the boundary. However, they noted that the tangential flux was incorrect near the surface, as is to be expected when the bounce-back rule is used. The issue of the tangential flux was addressed by Ginzburg [7], and it was noted that it is essential for the flux boundary conditions that there are no restrictions put on the tangential flux, at least to leading orders. The method presented in [7] is appealing, as it consists of only