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A lattice-Boltzmann scheme for Cattaneo's diffusion equation

José Alvarez-Ramírez, Francisco J. Valdés-Parada*, J. Alberto Ochoa-Tapia

División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Iztapalapa, Apartado Postal 55-534, Mexico D.F., 09340, Mexico

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Abstract

A lattice-Boltzmann (LB) formulation is developed for the simulation of Cattaneo's diffusion equation. To do this, the collision term is computed from a 1-step back relaxation dynamics which, in turn, induces a hyperbolic-type diffusion effect. The Fickian LB formulation is recovered in the limit as a relaxation time coefficient goes to zero.

Keywords: Lattice-Boltzmann; Cattaneo; Diffusion; Relaxation dynamics

1. Introduction

The LB method simulates physical transport phenomena with quasi-particles populating lattices [1,2]. The method is based on the idea that quasi-particles move across the lattice along links connecting neighboring lattice sites, and then undergo collisions upon arrival at a lattice site. For simulating physical phenomena, the collisions among particles must obey suitable physical laws. Thus, the fundamental problem of the LB method is to develop simplified kinetic models that incorporate the essential physics of microscopic processes so that the macroscopic averaged properties obey the desired laws [3,4]. Some applications of the LB method to diffusion problems have been reported in the literature. Ponce-Dawson et al. [5] first proposed a LB approach for reaction–diffusion processes. Wolf-Gladrow [6] derived a diffusion-based LB formulation for mathematical analysis of the problem showing that the introduction of a relaxation time coefficient enhances the stability properties of the simulation scheme.

In the Fickian diffusion model, the particle flux $N(x,t)$ is given by

$$N(x,t) = -D\partial_x \rho(x,t) \tag{1}$$

where $\rho(x,t)$ is the density of particles. For simplicity in notation, let ∂_x and ∂_t be the partial spatial and time differential operators $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial t}$, respectively. Together with the mass balance $\partial_t \rho(x,t) = -\partial_x N(x,t)$, the above equation yields

$$\partial_t \rho(x,t) = D\partial_x^2 \rho(x,t). \tag{2}$$

The parabolic nature of standard Fickian diffusion models leads to unphysical situations, such as infinite propagation velocities. Cattaneo's diffusion model is a hyperbolic equation with finite propagation velocity that

* Corresponding author. Tel.: +52 55 58044648; fax: +52 55 58044900.
E-mail address: iqfv@xanum.uam.mx (F.J. Valdés-Parada).

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is given as an extension of Fick's first law, Eq. (1). In fact, Cattaneo's constitutive equation is

$$t_r \partial_t N(x,t) + N(x,t) = -D\partial_x \rho(x,t) \tag{3}$$

where $t_r > 0$ is a given relaxation time coefficient. The corresponding diffusion equation is

$$t_r \partial_t^2 \rho(x,t) + \partial_t \rho(x,t) = D\partial_x^2 \rho(x,t). \tag{4}$$

Notice that the standard Fickian diffusion equation is recovered as $t_r \to 0$.

Statistically, Cattaneo's diffusion model can be derived from the Boltzmann equation [7,8]. The time-constant t_r is introduced into Cattaneo's equation to allow relaxation dynamics in the transport process. Physically, the time coefficient is related to the molecular relaxation processes that are occurring in the (crystalline or not) material's microstructure [9]. In this way, materials with more ordered microstructure, as in crystals, should display smaller relaxation time coefficients than materials with more disordered microstructures. As we will see in the next section, the time coefficient corresponds to the relaxation times of collisions of particles in a lattice.

Some applications of Cattaneo's equation include inflationary cosmological models [10], heat transfer in Bernard convection [11], and in the theory of diffusion in crystalline solids [12]. Given its physical importance, one is worried if Cattaneo's diffusion equation can be simulated by means of LB methods. This work focuses on this issue. An extended LB method is presented by proposing a dynamical collision function that introduces a type of memory effects in the diffusion process. The Fickian LB formulation is recovered in the limit as a relaxation time coefficient goes to zero.

2. Lattice-Boltzmann formulation for Cattaneo's equation

In order to concentrate in concepts rather than in algebraical manipulations, and for simplicity in presentation, we will focus on the one-dimensional case. Extensions to higher dimensional cases with different lattice geometries are straightforward.

The one-dimensional lattice case has two directions associated to the unit vectors $\mathrm{e}_1 = +1$ and $\mathrm{e}_2 = -1$. For each lattice node located at position x, and for time t, there is an associated particle distribution function $f_j(x,t)$, $j = 1, 2$. The distribution functions $f_1(x,t)$ and $f_2(x,t)$ refer to particles moving in the e_1 (*i.e.*, right) and e_2 (*i.e.*, left) directions, respectively. The LB equation for $f_j(x,t)$ is [3]

$$f_j\left(x + \Delta x \mathrm{e}_j, t + \Delta t\right) - f_j(x,t) = \Omega_j(x,t), \quad j = 1, 2 \tag{5}$$

where Δx and Δt are spatial and time scales, and $\Omega_j(x,t)$ is the so-called *collision function* depending of the distribution function $f_j(x,t)$. The following assumption is behind LB methods [3,5]. The distribution function $f_j(x,t)$ has appreciable variations only over a space scale $L \gg \Delta x$ and a time scale $T \gg \Delta t$. Under these assumptions, one can take the Taylor series expansion of the left hand side of Eq. (5) about $f_j(x,t)$ to obtain the following expression:

$$f_j\left(x + \Delta x \mathrm{e}_j, t + \Delta t\right) - f_j(x,t) = \sum_{k=1}^{\infty} \frac{1}{k!}\left(\Delta t \partial_t + \Delta x \mathrm{e}_j \partial_x\right)^k f_j(x,t). \tag{6}$$

Using the following normalized variables

$$y = \frac{x}{L}; \qquad \tau = \frac{t}{T} \tag{7}$$

allows us to rewrite Eq. (6) as follows:

$$\sum_{k=1}^{\infty} \frac{1}{k!}\left(\frac{\Delta t}{T}\partial_\tau + \frac{\Delta x}{L}\mathrm{e}_j \partial_y\right)^k \varphi_j(y,\tau) = \Psi_j(y,\tau) \tag{8}$$

where

$$\begin{aligned} \varphi_j(y,\tau) &\equiv f_j(Ly, T\tau) \\ \Psi_j(y,\tau) &\equiv \Omega_j(Ly, T\tau). \end{aligned} \tag{9}$$