Eur. Phys. J. Special Topics **171**, 245–249 (2009)

DOI: 10.1140/epjst/e2009-01035-5

THE EUROPEAN PHYSICAL JOURNAL SPECIAL TOPICS

Regular Article

The lattice Boltzmann advection-diffusion model revisited

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Abstract. Advection-diffusion processes can be simulated by the Lattice Boltzmann method. Two formulations have been proposed in the literature. We show that they are not fully correct (only first order accurate). A new formulation is proposed, which is shown to produce better results, both from the point of view of the Chapman-Enskog expansion or when comparing simulations with an exact time-dependent solution of the advection-diffusion equation.

1 Introduction

Advection-diffusion describes the diffusion of a quantity ρ subject to an external drift $\mathbf{u}$. It can be expressed by the differential equation

$$\partial_t \rho + \nabla(\mathbf{u}\rho) = D\nabla^2\rho \tag{1}$$

where $\mathbf{u}(\mathbf{r}, t)$ is a given function of space and time and D the diffusion coefficient.

Advection-diffusion processes are common, for instance, in fluid flow (passive scalar transported by a velocity field $\mathbf{u}(\mathbf{r}, t)$) or also in case of the diffusion of charged particles in presence of an electric field $\mathbf{E} = \mathbf{u}$.

The lattice Boltzmann (LB) method [1] provides a mesoscopic description of a physical system in terms of density distribution function $f_i(\mathbf{r}, t)$. The $f_i(\mathbf{r}, t)$ describe, on a discrete space-time world, the density of fluid particles entering site $\mathbf{r}$, at time t, with velocity $\mathbf{v}_i$, $i = 0, \ldots q-1$. In the so-called DdQq lattice (d-dimensional lattice with q velocities), the velocities $\mathbf{v}_i$ are chosen so that, in one time step Δt, a particle can reach one of its $q-1$ possible nearest neighbors. The velocity $\mathbf{v}_0 = 0$ describes particles at rest.

The quantity ρ is computed from the f_i by the relation $\rho = \sum_{i=0}^{q-1} f_i$.

The so-called single-time relaxation LB model reads

$$f_i(r + \Delta t\mathbf{v}_i,\ t + \Delta t) = \left(1 - \frac{1}{\tau}\right) f_i + \frac{1}{\tau} f_i^{eq} \tag{2}$$

where f_i^{eq} is a given function of ρ (and possibly higher moments of f_i). The quantity τ is a relxation time, which can be adjusted to tune the transport coefficients.

By choosing an adequate expression of f_i^{eq}, the LB approach has been successfully used to describe many phenomena such as complex flows, reaction-diffusion processes or wave equation [2]. Advection-diffusion processes have also been addressed within the LB framework.

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However, two different expressions for f_i^{eq} can be found in the literature. For instance in [3–5], we find

$$f_i^{eq} = t_i \rho \left(1 + \frac{1}{c_s^2} \mathbf{v}_i \cdot \mathbf{u}\right) \tag{3}$$

where t_i and c_s^2 are some constants such that

$$\sum_{i=0}^{q-1} t_i = 1 \quad \sum_{i=0}^{q-1} t_i v_{i\alpha} v_{i\beta} = c_s^2 \delta_{\alpha\beta} \tag{4}$$

where greek indices label spatial coordinates.

In other papers (see for instance [6–8]), the following expression is used for f_i^{eq}

$$f_i^{eq} = t_i \rho \left(1 + \frac{1}{c_s^2} \mathbf{v}_i \cdot \mathbf{u} + \frac{1}{2c_s^4} Q_{i\alpha\beta} u_\alpha u_\beta\right) \tag{5}$$

where $Q_{i\alpha\beta}$ is defined as $Q_{i\alpha\beta} = v_{i\alpha} v_{i\beta} - c_s^2 \delta_{\alpha\beta}$ (here we follow Einstein summation convention over repeated greek indices.)

In this paper we show that none of these expressions guarantees that the LB model reproduces the advection-diffusion equation (1) to second order accuracy in Δt, the time step, and Δr, the lattice spacing.

The paper is organized as follows. In section 2, we derive the PDE associated with eq. (2) for both expressions (3) and (5). We show the presence of a term absent in eq. (1). We indicate how it can be eliminated by modifying eq. (2) by adding a body force. In section 3 we validate the theoretical findings with a time-dependent advection-diffusion problem which can be solved analytically and simulated with the LB approach. Some conclusions are drawn in section 4.

2 The Lattice Boltzmann advection-diffusion model

2.1 The Chapman-Enskog solution

Let us now assume that the local equilibrium is choosen as

$$f_i^{eq} = t_i \rho \left(1 + \frac{1}{c_s^2} \mathbf{v}_i \cdot \mathbf{u} + \eta \frac{1}{2c_s^4} Q_{i\alpha\beta} u_\alpha u_\beta\right) \tag{6}$$

where η is a quantity which is either 1 or 0, whether we are interested in expressions (3) or (5) of f_i^{eq}.

Then, a first-order multiscale Chapman-Enskog expansion (see [2,9]) applied on eq. (2) gives the following equation for ρ

$$\partial_t \rho + \nabla(\mathbf{u}\rho) = D\nabla^2 \rho + \frac{D}{c_s^2} \partial_t \nabla(u\rho) + \eta \frac{D}{c_s^2} \partial_\alpha \partial_\beta \rho u_\alpha u_\beta. \tag{7}$$

Note that the above derivation is second order accurate in Δt and Δr. With respect to eq. (1) the proposed LB approaches contain the following unwanted term Δ

$$\Delta = \frac{D}{c_s^2} \left[\partial_t \nabla(u\rho) + \eta \partial_\alpha \partial_\beta \rho u_\alpha u_\beta\right]. \tag{8}$$

2.2 Case of a linear local-equilibrium

For $\eta = 0$, f^{eq} is linear in $\mathbf{u}$. Eq. (8) reduces to $\Delta = (D/c_s^2)\partial_t \nabla(u\rho)$. To interprete this term, let us assume that $\mathbf{u}$ is constant. By taking the gradient of eq. (7) and neglecting all third order derivatives, we obtain

$$\partial_t \nabla \rho + \mathbf{u}\nabla^2 \rho = 0. \tag{9}$$

Thus, the error term can be written as $\Delta = -(D/c_s^2)u^2\nabla^2\rho$ and this means that eq. (7) become

$$\partial_t \rho + \mathbf{u} \cdot \nabla \rho = D\left(1 - \frac{u^2}{c_s^2}\right)\nabla^2\rho. \tag{10}$$

Therefore, the error terms amounts to a undesired correction to the diffusion coefficient, proportional to the square of the advection velocity. From eq. (4), c_s is parameter of the LB model which has the unit of a velocity, i.e. it scales as $\bar{c}_s(\Delta r/\Delta t)$, where $\bar{c}_s$ is a pure number. The quantities D and $\mathbf{u}$ are assumed to be given by the physical problem. As such they are independent of the chosen time and space discretization Δr and Δt. Thus, the correction (10) to the diffusion coefficient scales as $(\Delta t/\Delta r)^2$. Thus, reducing Δr while keeping Δt constant increases the error and should be avoided. If we take both the limits $\Delta t \to 0$ and $\Delta r \to 0$, with $\Delta r^2/\Delta t$ constant (natural limit for a diffusion process), then the correction to the diffusion coefficient is $\mathcal{O}(\Delta r)$. The scheme is thus first order accurate. But, if we take $\Delta t \to 0$, $\Delta r \to 0$ and $\Delta r/\Delta t$ constant, then the error is $\mathcal{O}(1)$ and the scheme is zeroth order accurate.

2.3 Case of a non-linear local-equilibrium

Let us now consider the case $\eta = 1$, corresponding to the non-linear expression of f^{eq} in $\mathbf{u}$. Eq. (8) can be written as

$$\begin{aligned}\Delta &= \frac{D}{c_s^2}\partial_\alpha\left[\partial_t\rho u_\alpha + \eta\partial_\beta\rho u_\alpha u_\beta\right] = \frac{D}{c_s^2}\partial_\alpha\left[(u_\alpha\partial_t\rho + \rho\partial_t u_\alpha) + \eta\left(u_\alpha\partial_\beta\rho u_\beta + \rho u_\beta\partial_\beta u_\alpha\right)\right] \\ &= \frac{D}{c_s^2}\partial_\alpha\left[u_\alpha\left(\partial_t\rho + \eta\partial_\beta\rho u_\beta\right) + \rho\left(\partial_t u_\alpha + \eta u_\beta\partial_\beta u_\alpha\right)\right].\end{aligned} \tag{11}$$

Since ρ obeys eq. (7) $\partial_\alpha[\partial_t\rho + \eta\partial_\beta\rho u_\beta]$ can be neglected as it amounts to a third order derivative. Therefore, the error term is

$$\Delta = \frac{D}{c_s^2}\partial_\alpha\left[\rho(\partial_t u_\alpha + u_\beta\partial_\beta u_a)\right]. \tag{12}$$

In many applications of the advection-diffusion equation, the advection is due to a fluid flow. In the case $\mathbf{u}$ obeys the incompressible Navier-Stokes equation, the term Δ can be further developed. We then have

$$(\partial_t u_\alpha + u_\beta\partial_\beta u_a) = -\frac{1}{\rho_f}\partial_\alpha p_f + \nu\partial_\beta^2 u_\alpha$$

where ρ_f and p_f are the density and pressure of the advecting fluid and ν its viscosity.

We can neglect $\nu\partial_\beta^2 u_\alpha$ because it will contribute to a third order derivative. Then

$$\Delta = -\frac{D}{c_s^2}\partial_\alpha\left[\frac{\rho}{\rho_f}\partial_\alpha p_f\right]. \tag{13}$$

2.4 A proposed correction

In the case we consider f^{eq} linear in $\mathbf{u}$ (i.e. eq. (3)), only the linear component is present in the unwanted term Δ. It can be canceled by adding a term

$$F_i = \frac{\mathbf{v}_i}{c_s^2} t_i \left(1 - \frac{1}{2\tau}\right) \partial_t(\rho\mathbf{u}) \tag{14}$$

on the right hand side of the LB evolution equation (2) as a "body force" (see [9]). This recovers second order accuracy in time and space. This body force term can be obtained, to the required level of accuracy, by the finite difference expression

$$\partial_t(\rho u) \approx \rho(t)u(t) - \rho(t-1)u(t-1).$$

When considering the non-linear form (5), the full expression of Δ cannot be canceled through a "body force", unless $\mathbf{u}$ has additional properties. Thus, in general, the approach would be first to cancel the non-linear contribution in f^{eq} and then apply the "linear" correction discussed above. However, when the external velocity field is solution to the incompressible Navier-Stokes equations, the unwanted term described by eq. (13) can be cancelled in a simple way with the following correction term

$$F_i = -\frac{\mathbf{v}_i}{c_s^2} t_i \left(1 - \frac{1}{2\tau}\right) \frac{\rho}{\rho_f} \nabla p_f. \tag{15}$$

3 Numerical results

Eq. (1) can be solved analytically in the case of a periodic 1D system of length L, where the driving velocity is

$$u(x,t) = u_0 \cos(\nu t). \tag{16}$$

Note that this advection field is solution of the Navier-Stokes equation in a periodic domain, when a time-dependent pressure gradient (or body force) $\nabla p \propto \sin(\nu t)$ is applied.

If we consider for instance the initial condition $\rho(x,0) = \rho_0 + \rho_1 \cos kx$, for $x \in [0,L]$ and $k = (2\pi n)/L$, then the time-dependent solution of the periodic 1D advection-diffusion equation is easily found to be

$$\rho = \rho_0 + \rho_1 e^{-k^2 Dt}[\cos kx \cos(u_0(k/\nu)\sin \nu t) + \sin kx \sin(u_0(k/\nu)\sin \nu t)]. \tag{17}$$

We can now compare the result of simulations against the analytical solution. After one period $T = \frac{1}{\nu} = N_t \Delta t$, where N_t is the number of time steps in one period, the error is computed as $\epsilon^2 = (\sum_t \sum_x |\rho_{simulation} - \rho_{analytical}|^2)/(N_x N_t)$ with N_x the number of grid points. From eq. (10) we expect that the errors will grow as u_0 increases, as shown in fig. 1. We observe that the proposed corrections improve the quality of the simulations. However, when $\mathbf{u}$ obeys Navier-Stokes, the non-linear f^{eq} performs better than the linear f^{eq}. In this case, it is also found that the value of c_s^2 affects the accuracy ($c_s^2 = 1/3$ being the best here) whereas, when eq. (3) is used, c_s can be chosen much more arbitrarily.

Fig. 1 also illustrates how accuracy changes when refining the space, with fixed Δt. As discussed above, refining space without refining time eventually degrades the precision.

4 Conclusion

Two different expressions of f^{eq} are found in the literature to model an advection-diffusion process with the LB method. We have shown that none of them is fully correct. However, adding a simple correction term, acting as a body force, improves the accuracy of the LB advection-diffusion model to second order in Δt and Δr. The two formulations should be used

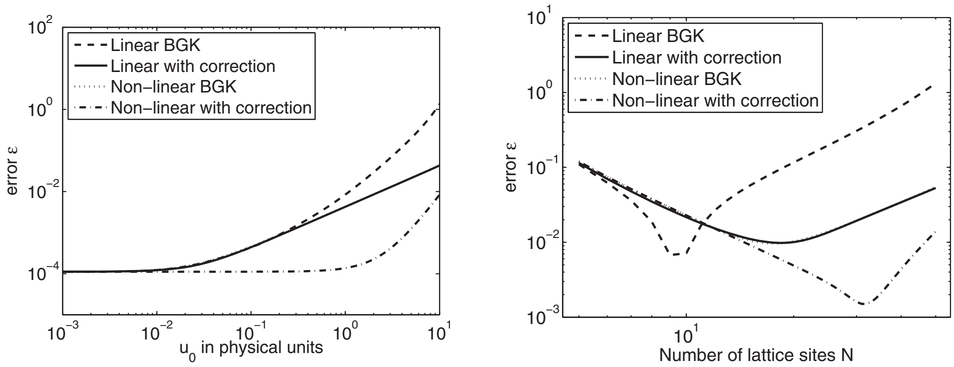

Fig. 1. Error when comparing LB simulations with the analytical solution of the advection-diffusion equation. Left: the amplitude u_0 of the external velocity term is varied, whereas the number of lattice sites $N = 40$ and the time discretization $\delta_t = 0.002$ are constant. Right: the number of lattice sites is varied, whereas the velocity amplitude $u_0 = 8.0$ and the time discretization $\delta_t = 0.002$ are constant. The curves for the corrected linear model and for the uncorrected non-linear model are almost identical.

in different situations. If the advecting field $\mathbf{u}$ is solution to the Navier-Stokes eq. then the non-linear version of f^{eq} should be used, with a correction term proportional to ∇p_f. If $\mathbf{u}$ does not obey Navier-Stokes, the linear f^{eq} should be preferred, with a correction term proportional to $\partial_t(\rho\mathbf{u})$. Our study also shows the importance of correctly taking the limit $\Delta t \to 0$ and $\Delta r \to 0$. For instance refining the space while keeping the time discretization constant can actually degrade the quality of the simulation instead of improving it [9].

We thank Alexander Wagner for pointing us the role of the u^2 term in the local equilibrium distribution, when the advection field u is solution of the Navier-Stokes equation. We also thank him for sharing with us his calculations, which are partly reproduced above. The work presented here was supported by the Swiss National Science Foundation (FN 200020–1007931, PBGe2–117144) and the European project COAST.

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