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A Lattice Boltzmann Equation for Diffusion

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The formulation of lattice gas automata (LGA) for given partial differential equations is not straightforward and still requires "some sort of magic." Lattice Boltzmann equation (LBE) models are much more flexible than LGA because of the freedom in choosing equilibrium distributions with free parameters which can be set after a multiscale expansion according to certain requirements. Here a LBE is presented for diffusion in an arbitrary number of dimensions. The model is probably the simplest LBE which can be formulated. It is shown that the resulting algorithm with relaxation parameter $\omega = 1$ is identical to an explicit finite-difference (EFD) formulation at its stability limit. Underrelaxation ($0 < \omega < 1$) allows stable integration beyond the stability limit of EFD. The time step of the explicit LBE integration is limited by accuracy and not by stability requirements.

KEY WORDS: Diffusion; finite differences; lattice Boltzmann equation; underrelaxation; numerical stability; explicit schemes.

1. INTRODUCTION

The last 10 years have seen a rapid development of new numerical methods for the solution of partial differential equations, especially Navier–Stokes equations. After the proposal of the first successful lattice gas automata (LGA) for hydrodynamics in two dimensions by Frisch *et al.*,[8] several new LGA models have been presented each year and applied to various problems, among them hydrodynamics in three dimensions,[7, 17] flow through porous media,[20] immiscible fluids,[21] several fluids and external forces,[13] magnetohydrodynamics,[3, 16, 4] and diffusion-reaction equations,[6, 12] to name only a few.

Lattice Boltzmann equations (LBE) have been used as an analytical tool in the theory of LGA (see, for example, Frisch *et al.*[8]). In 1988,

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McNamara and Zanetti[15] proposed LBE as a numerical scheme. The first LBE models were still plagued by similar problems to LGA (breaking of Galilei invariance, pressure depending explicitly on flow speed) due to Fermi–Dirac distribution functions and certain underlying grids. It took some years to develop a generation of LBE based on different distribution functions, multispeed grids, and tunable parameters (BGK models, see below; see, for example, Martinez *et al.*[14] and references therein).

The creation of LGA for certain partial differential equations still seems to require "some sort of magic."[22] Here a simple LBE model for diffusion is presented and it is shown how straightforward it is to derive such a model. In addition, the resulting algorithms are compared with an explicit finite-difference (EFD) scheme.

2. FINITE-DIFFERENCE APPROXIMATION

An explicit finite-difference scheme for the diffusion equation

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T$$

(T is the concentration of a tracer, κ is the diffusion coefficient, and ∇^2 is the Laplace operator in D dimensions in Cartesian coordinates) results from forward approximation in time and central differences in space,

$$\begin{aligned} T^{(n+1)}_{k_1,k_2,\ldots,k_D} = \frac{\kappa\,\Delta t}{(\Delta x)^2}\,(&T^{(n)}_{k_1+1,k_2,\ldots,k_D} + T^{(n)}_{k_1-1,k_2,\ldots,k_D} \\ &+ \cdots + T^{(n)}_{k_1,k_2,\ldots,k_D+1} + T^{(n)}_{k_1,k_2,\ldots,k_D-1}) \\ &+ \left(1 - 2D\frac{\kappa\,\Delta t}{(\Delta x)^2}\right) T^{(n)}_{k_1,k_2,\ldots,k_D} \end{aligned}$$

where equidistant and equal spacing in all dimensions has been assumed. The scheme is stable for

$$0 < \Delta t \leqslant \frac{1}{2D}\frac{(\Delta x)^2}{\kappa}$$

(see, for example, Ames[1]). At the upper stability limit the scheme becomes especially simple,

$$\begin{aligned} T^{(n+1)}_{k_1,k_2,\ldots,k_D} = (&T^{(n)}_{k_1+1,k_2,\ldots,k_D} + T^{(n)}_{k_1-1,k_2,\ldots,k_D} \cdots \\ &+ T^{(n)}_{k_1,k_2,\ldots,k_D+1} + T^{(n)}_{k_1,k_2,\ldots,k_D-1})/(2D) \end{aligned}$$

that is, T at the new time level is given by the mean over all neighbor values at the previous time level.

3. THE LATTICE BOLTZMANN EQUATION FOR DIFFUSION

"... it is well known that 90° rotational invariance is sufficient to yield full isotropy for *diffusive* phenomena."[22]

According to Toffoli and Margulos,[22] it is sufficient to use a square or a cubic lattice in two or three dimensions, respectively. The following model is applicable in an arbitrary number of dimensions. The grid velocities (vectors connecting neighboring grid points) are defined by

$$\mathbf{c}_{2n-1} = (0, 0, \ldots, 0, 1, 0, \ldots, 0), \qquad \mathbf{c}_{2n} = (0, 0, \ldots, 0, -1, 0, \ldots, 0), \quad n = 1, 2, \ldots, D$$

where D is the dimension.

In general, the equilibrium distributions $T_m^{(0)}$ depend on the conserved quantities (here only T), a number of parameters $\gamma_k (k = 0, 1, \ldots, N)$, and the direction (index m). Here, grids with only one speed are considered and the equilibrium distribution functions $T_m^{(0)}$ do not depend on m. T is given as the sum over the distribution functions T_m,

$$T(\mathbf{x}, t) = \sum_m T_m(\mathbf{x}, t) = \sum_m T_m^{(0)}(\mathbf{x}, t) \tag{1}$$

where the summation runs over all directions ($m = 1, 2, \ldots, M = 2D$).

The diffusion equation is a linear differential equation. Hence it is reasonable to use a linear ansatz for $T_m^{(0)}$,

$$T_m^{(0)} = \gamma_0 + \gamma_1 T \tag{2}$$

Inserting (2) into (1) yields

$$T_m^{(0)} = \frac{T}{2D}$$

that is, all free parameters are already fixed by the definition of the tracer concentration. The diffusion coefficient κ will result from multiscale expansion as described below.

3.1. Multiscale Expansion

The LBE model is defined by the grid, the equilibrium distribution $T_m^{(0)}$ and the kinetic equation

$$T_m(\mathbf{x}+\mathbf{c}_m, t+1) = (1-\omega)\, T_m(\mathbf{x}, t) + \omega T_m^{(0)}(\mathbf{x}, t) \tag{3}$$

which states that the distribution at the new time level $(t+1)$ at the neighboring site $(\mathbf{x}+\mathbf{c}_m)$ is a weighted sum of the distribution $T_m(\mathbf{x}, t)$ and the equilibrium distribution $T_m^{(0)}(\mathbf{x}, t)$. Models with parameter ω go under various names: enhanced collision,[11] BGK (after Bhatnagar, Gross, and Krook[2]), STRA (single-time relaxation approximation[5]), or SOR (successive overrelaxation[18]). The LBE model is stable for $0<\omega<2$. Now the macroscopic equations will be derived by a multiscale analysis (compare Frisch *et al.*[9] for an analogous procedure for LGA). The distribution functions are expanded up to linear terms in the small expansion parameter ε,

$$T_m = T_m^{(0)} + \varepsilon T_m^{(1)} + \mathcal{O}(\varepsilon^2)$$

From the kinetic equation (3) one can calculate an approximation of $T_m^{(1)}$,

$$\begin{aligned} T_m(\mathbf{x}+\mathbf{c}_m, t+1) &= T_m(\mathbf{x}, t) + \partial_{x_\alpha} c_{m\alpha} T_m + \partial_t T_m + \mathcal{O}(\varepsilon^2) \\ &= (1-\omega) \underbrace{T_m(\mathbf{x}, t)}_{= T_m^{(0)} + \varepsilon T_m^{(1)} + \mathcal{O}(\varepsilon^2)} + \omega T_m^{(0)}(\mathbf{x}, t) \end{aligned}$$

$$\rightarrow$$

$$\varepsilon T_m^{(1)} = -\frac{1}{\omega} \partial_{x_\alpha} c_{m\alpha} T_m - \frac{1}{\omega} \partial_t T_m + \mathcal{O}(\varepsilon^2)$$

Diffusion is a slow process on large spatial scales, which suggests the following scaling (same as for the derivation of the Navier–Stokes equations in Frisch *et al.*[19]):

$$\partial_t \rightarrow \varepsilon^2 \partial_{t_2}$$

$$\partial_{\mathbf{x}} \rightarrow \varepsilon \partial_{\mathbf{x}_1}$$

The components of the grid velocities obey the following equations:

$$\sum_m \mathbf{c}_m = 0$$

$$\sum_m c_{m\alpha} c_{m\beta} = 2\delta_{\alpha\beta}$$

and therefore

$$\sum_m \mathbf{c}_m T_m^{(0)} = \frac{T}{2D} \sum_m \mathbf{c}_m = 0$$

Inserting the expansion and the scalings into the conservation relation for tracer concentration, one gets up to second order in ε

$$\begin{aligned} 0 &= \sum_m [T_m(\mathbf{x} + \mathbf{c}_m, t+1) - T_m(\mathbf{x}, t)] \\ &= \sum_m [T_m(\mathbf{x}, t) + \underbrace{\varepsilon^2 \partial_{t_2} T_m}_{\to \partial_t T} + \varepsilon \partial_{x_{1\alpha}} c_{m\alpha} T_m + \tfrac{1}{2} \varepsilon^2 \partial_{x_{1\alpha}} \partial_{x_{1\beta}} c_{m\alpha} c_{m\beta} T_m^{(0)} \\ &\quad - T_m(\mathbf{x}, t) + \mathcal{O}(\varepsilon^3)] \end{aligned}$$

and

$$\begin{aligned} \sum_m \varepsilon \partial_{x_{1\alpha}} c_{m\alpha} T_m &= \varepsilon \partial_{x_{1\alpha}} \underbrace{\sum_m c_{m\alpha} T_m^{(0)}}_{=0} + \sum_m \varepsilon^2 \partial_{x_{1\alpha}} c_{m\alpha} T_m^{(1)} + \mathcal{O}(\varepsilon^3) \\ &= -\frac{1}{\omega} \sum_m \varepsilon^2 \partial_{x_{1\alpha}} \partial_{x_{1\beta}} c_{m\alpha} c_{m\beta} T_m^{(0)} + \mathcal{O}(\varepsilon^3) \\ &= -\frac{1}{\omega} \frac{1}{D} \underbrace{\varepsilon^2 \delta_{\alpha\beta} \partial_{x_{1\alpha}} \partial_{x_{1\beta}} T}_{\to \nabla^2 T} + \mathcal{O}(\varepsilon^3) \end{aligned}$$

$$\sum_m \frac{1}{2} \varepsilon^2 \partial_{x_{1\alpha}} \partial_{x_{1\beta}} c_{m\alpha} c_{m\beta} T_m^{(0)} = \frac{1}{2D} \varepsilon^2 \delta_{\alpha\beta} \partial_{x_{1\alpha}} \partial_{x_{1\beta}} T$$

and finally

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T$$

with

$$\kappa = \left(\frac{1}{\omega} - \frac{1}{2} \right) \frac{1}{D}$$

3.2. The Special Case $\omega = 1$

For $\omega = 1$ the kinetic equation (3) reduces to

$$T_m(\mathbf{x} + \mathbf{c}_m, t+1) = T_m^{(0)}(\mathbf{x}, t)$$

and the diffusion coefficient is $\kappa = 1/(2D)$. This LBE model is identical to the finite-difference scheme at the stability limit. The right-hand side of the kinetic equation is just the mean value of the nearest-neighboring sites and the diffusion coefficient is the maximal value allowed by the stability condition. For the LBE model the diffusion coefficient is expressed in the units $\Delta t = \Delta x = 1$; the diffusion coefficient at the stability limit of the EFD reads

$$\kappa = \frac{1}{2D}\frac{(\Delta x)^2}{\Delta t} = \frac{1}{2D}$$

This scheme requires only two arrays in memory: the tracer concentrations at two time levels.

3.3. The General Case

In the general case one has to store $M = 2D$ distributions in addition to the tracer concentrations at two time levels. What do we gain from this

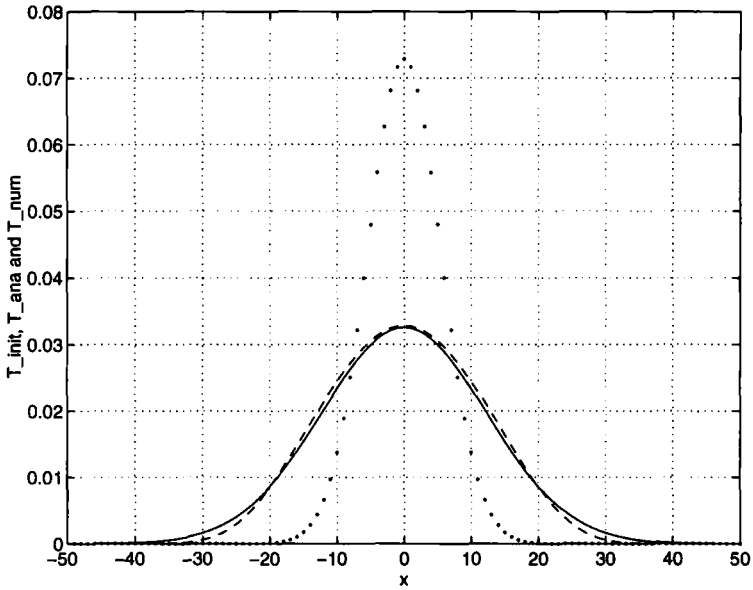

Fig. 1. Integration of the diffusion equation in one dimension by the BGK-LBE with $\omega = 0.3$. The integration starts at time $t_i = 15/\kappa(\omega)$ with initial values $T(x, t_i) = [1/2(\pi\kappa t_i)^{1/2}]$ $\exp(-x^2/4\kappa t_i)$ (dotted line) and ends at $t_f = 75/\kappa(\omega)$. The figure shows the numerical results (broken line) together with the analytical solution (solid line).

extra cost? In the range $0 < \omega < 1$ (underrelaxation) the diffusion coefficient κ is larger than the value at the stability limit of the EFD scheme, while we still keep $\Delta t = \Delta x = 1$. In contrast to EFD, the LBE model is stable in this parameter range.

3.4. Numerical Experiments

To test the predictions of the LBE model outlined above the one-dimensional diffusion equation was integrated. As initial conditions, values of an analytical solution were used, namely

$$T(x, t_i) = \frac{1}{2(\pi\kappa t_i)^{1/2}} \exp\left(-\frac{x^2}{4\kappa t_i}\right)$$

The integration starts at $t_i = 15/\kappa(\omega)$ and ends at $t_f = 75/\kappa(\omega)$; thus the time interval depends on $\kappa(\omega)$, but in each case the integration starts with the same numerical values and ends after the maximum decreases from ~ 0.073 to ~ 0.033. Figure 1 shows the results of such an integration for $\omega = 0.3$ together with the analytical solution and the initial values. By

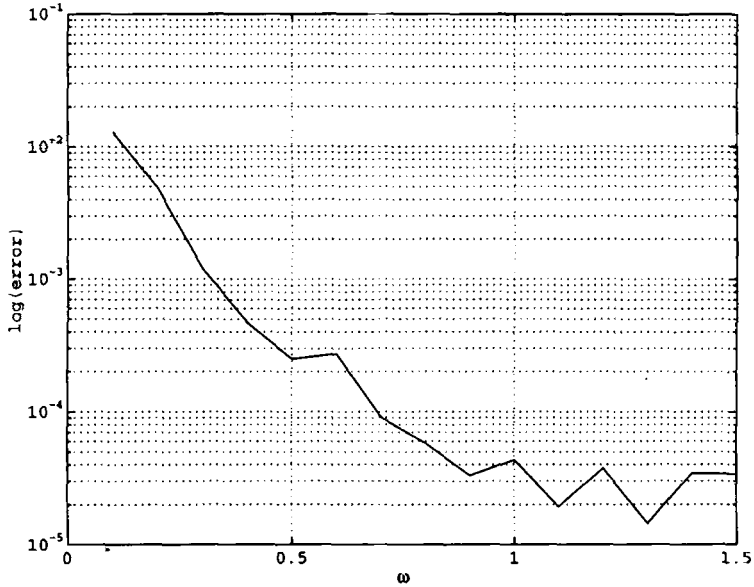

Fig. 2. Integration of the diffusion equation in one dimension by the BGK-LBE. The integration starts at time $t_i = 15/\kappa(\omega)$ with initial values $T(x, t_i) = [1/2(\pi\kappa t_i)^{1/2}] \exp(-x^2/4\kappa t_i)$ and ends at $t_f = 75/\kappa(\omega)$. The plot shows the logarithm of the maximum error ($\max\{|T_{\text{numerical solution}} - T_{\text{analytical solution}}|\}$) at the end of the integrations as a function of ω. The error increases at small values of ω (large values of the diffusion coefficients).

appropriate choice of ω, one can keep $\Delta t = 1$ for "arbitrarily" large diffusion coefficients: the scheme is stable but the numerical error increases with increasing diffusion coefficient (compare Fig. 2). Thus, we have an explicit scheme (BGK-LBE) where the length of the time step is no longer limited by stability requirements. The large error at small values of ω stems from the fact that explicit approximations of parabolic equations act like a hyperbolic system with two real finite-difference characteristics instead of only a single real characteristic of the continuous system.[1]

4. SUMMARY AND CONCLUSION

A very simple LBE for diffusion in an arbitrary number of dimensions is proposed. For $\omega = 1$ the resulting algorithm is identical to an explicit finite-difference scheme at its stability limit. Thus the LBE scheme is not only stable, but automatically picks the maximal allowed diffusion coefficient κ to ensure stability of the EFD scheme.

For LGA the transport coefficients depend on the collision rules, which are never optimal, in the sense that they yield only a certain approximation of the (continuous) local equilibrium functions (compare the various FHP models with and without rest particles in Frisch *et al.*[9] or the various collision rules proposed for FCHC by Hénon,[10] Rem and Somers,[19] and van Coevorden *et al.*[23]), whereas for LBE, the collisions (which do not show up explicitly) can create local equilibrium at each time step. By reducing the number of collisions in LGA one gets models with higher diffusion coefficients while stability is assured. This can be regarded as a kind of underrelaxation.

In the BGK-LBE model the diffusion coefficient κ; is an adjustable parameter. Of special interest is the parameter range $0 < \omega < 1$. The use of information contained in the nonequilibrium distribution functions allows explicit stable integration beyond the stability limit of the EFD scheme. Thus, the time step is limited by accuracy and not by stability requirements.

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NOTE ADDED IN PROOF

The LBE model can be generalized by introducing a tracer dependent iteration parameter $\omega(T)$. An analogous multiscale analysis yields the diffusion equation

$$\frac{\partial T}{\partial t} = \nabla[\kappa(T)\,\nabla T]$$

with a diffusion coefficient which depends on the concentration T

$$\kappa(T) = \left[\frac{1}{\omega(T)} - \frac{1}{2}\right]\frac{1}{D}$$

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