Hydrodynamic behaviour of Lattice Boltzmann and Lattice BGK models

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Abstract

We present a numerical analysis of the validity of classical and generalized hydrodynamics for Lattice Boltzmann Equation (LBE) and Lattice BGK methods in two and three dimensions, as a function of the collision parameters of these models. Our analysis is based on the wave-number dependence of the evolution operator. Good ranges of validity are found for BGK models as long as the relaxation time is chosen smaller than or equal to unity. The additional freedom in the choice of collision parameters for LBE models does not seem to give significant improvement.
Recently, Lattice-gas Automata (LGA) methods have been developed as a new computational approach to fluid dynamics [1]. Using purely local Boolean operations to represent particle collisions, they have proved to be extremely efficient, although, due to the fluctuations inherent in the method, statistical averaging is necessary in order to extract information. The Lattice Boltzmann Equation (LBE) [2] and Lattice BGK method [3] [4], by using continuous distribution functions, eliminate this statistical noise and offer significant computational advantages.

It is important to define ways in which these methods can be optimized. In the past, since one of the main applications has been the study of flows at high Reynolds number, it has been customary to minimize the viscosity by tuning the parameters of the collision operators. However, since applications to low Reynolds number flows are becoming increasingly important [5] [6], other criteria might be used. In particular, it is of interest to define the spatial scale for which the models reproduce hydrodynamics, and how this scale depends upon the parameters of the simulation.

This analysis was first considered by Luo et al. [7], and developed by Grosfils et al. [8] and Das and Ernst [9] for the study of LGA’s. They show [9] that some of the simplest LGA models reproduce classical or even generalised hydrodynamics [9] only over very large spatial scales, and point out that observations in the literature of “negative viscosities” [10] can be traced to those scale effects. Since, however, there have been no similar investigations of LBE or BGK methods, we present in this letter a numerical analysis of the validity of hydrodynamics for these methods in two and three dimensions, the latter being an extension of the analysis of four-dimensional models based on the FCHC lattice [1].

In the LBE with enhanced collisions [11], the collision operator is linearized around the equilibrium distribution function to give the kinetic equation:

\[ f_\alpha(x + c_\alpha, t + 1) = f_\alpha(x, t) + \sum_{\beta=1}^{b} \Omega_{\alpha\beta} [f_{\beta}(x, t) - f_{\beta}^{\text{equil}}(x, t)] \]  

(1)

where \( \Omega_{\alpha\beta} \) is the linearized collision operator, \( f_\alpha(x, t) \) is the occupation number of velocity \( c_\alpha \) at node \( x \) and time \( t \), \( f_{\beta}^{\text{equil}}(x, t) \) is the chosen equilibrium distribution function and \( b \) the number of velocity directions. By symmetry, the matrix element \( \Omega_{\alpha\beta} \) depends only on the angle \( \theta \) between the directions \( \alpha \) and \( \beta \), and by convention is given the value \( a_\theta \) [11]. In two dimensions, for a single speed
model based on the hexagonal lattice [4] (6 velocity directions), there are four possible matrix elements, $a_0$, $a_{60}$, $a_{120}$ and $a_{180}$ while for the four dimensional FCHC lattice (24 velocity directions), there are five possible matrix elements, $a_0$, $a_{60}$, $a_{90}$, $a_{120}$ and $a_{180}$. The conditions of mass and momentum conservation then reduce the number of independent matrix elements, leaving two and three such elements for the two and four dimensional situations respectively.

Linear stability analysis requires that the eigenvalues of $\Omega$ be contained in the interval $(-2,0)$. This places further restrictions on the matrix elements, which can be made explicit by writing the non-zero eigenvalues as [11]:

$$\lambda = 6(a_0 + a_{60})$$
$$\sigma = -6(a_0 + 2a_{60})$$

in two dimensions, with multiplicities 2 and 1 respectively, and

$$\lambda = a_0 - 2a_{90} + a_{180}$$
$$\sigma = 3(a_0 - a_{180})/2$$
$$\gamma = 3(a_0 + 6a_{90} + a_{180})/2$$

in four dimensions, with multiplicities 9, 8 and 2 respectively. It is also useful to note that the eigenvalue $\lambda$ is linked to the kinematic viscosity of the fluid by [11]

$$\nu = -\frac{c^2}{d+2}\left(\frac{1}{\lambda} + \frac{1}{2}\right)$$

where $d$ is the dimensionality of the simulation. The eigenvalues $\sigma$ in two dimensions and $\sigma$ and $\gamma$ in four dimensions control the decay of the so-called ghost fields [2], and therefore a preferred choice for their values is $-1$, forcing a rapid decay of these unphysical fields.

The BGK model (so-called in analogy with the BGK treatment of the Boltzmann equation [12]) is a further simplification of the LBE model, whereby the collision part of the kinetic equation is parameterised by a single relaxation parameter $\tau$ such that [3] [4]:

$$f_\alpha(x + c_\alpha, t + 1) = f_\alpha(x, t) - \tau^{-1} \cdot [f_\alpha(x, t) - f_\alpha^{equil}(x, t)].$$

(2)

The relaxation parameter $\tau$ (which linear stability requires to be larger than 1/2, $1/2 < \tau < 1$ being called subrelaxation and $\tau > 1$ over-relaxation) is linked to
the kinematic viscosity by the relation \[3\]

\[\nu = \frac{c^2(2\tau - 1)}{2(d+2)}.\]

The value \(\tau = 1\) plays the same role as \(\sigma = \gamma = -1\) in the LBE model since it relaxes the distribution function \(f_\alpha(x,t)\) to its equilibrium \(f^\text{equil}_\alpha(x,t)\) in a single time step.

To analyse the hydrodynamic behaviour of these models, we use the properties of the evolution operator \(H(k)\) \[7\]. Thus, if \(\phi_\alpha(x,t)\) is the deviation of \(f_\alpha(x,t)\) from the equilibrium distribution,

\[\phi_\alpha(x,t) = f_\alpha(x,t) - f^\text{equil}_\alpha(x,t),\]

\(H(k)\) can be defined by Fourier transforming the kinetic equation (1) such that \[7\]:

\[|\phi(k, t+1)> = H(k)|\phi(k,t)> .\]

Here, \(\langle c_\alpha|\phi(k,t) >= \phi_\alpha(k,t)\), \(H(k) = D(k)H(0)\), and \(H(0) = I + \Omega\), where \(I\) is the unit matrix, and the displacement operator \(D(k)\) is the diagonal matrix \(\text{diag}[\exp(-ik \cdot c_1), \exp(-ik \cdot c_2), \ldots, \exp(-ik \cdot c_b)]\). The eigenvalues of \(H(k)\), defined from

\[H(k)|\psi_\lambda(k)> = e^{z_\lambda(k)}|\psi_\lambda(k)>\]

then give information about the transport coefficients corresponding to the collision matrix \(\Omega\).

In the long-wavelength regime \((k \to 0, \text{ where } k = |k|)\), two types of modes exist: hydrodynamic modes, related to the conservation laws, with \(\text{Re}[z_\lambda(k)] \sim O(k^2)\), and rapidly decaying kinetic modes, with \(\text{Re}[z_\lambda(k)] < 0\), without any physical significance. Transport coefficients are related to the hydrodynamic modes \[3\]. In a model without explicit energy conservation in two (four) dimensions three (five) such modes exist, two (two) propagating but damped sound modes \(\lambda = \pm\) and one (three) diffusive shear modes \(\lambda = \perp\), with \(\text{Im}[z_\perp(k)] = 0\). The real part \(\text{Re}[z_\lambda(k)]\) represents damping, and if the imaginary part \(\text{Im}[z_\lambda(k)] = \pm c_s(k)k\) is nonvanishing, the mode propagates with speed \(c_s(k)\) \[9\]. The wave-vector dependent kinematic shear viscosity is defined as \[3\]

\[\nu(k) \equiv -z_\perp(k)/k^2.\]
while the sound damping constant is defined as

\[ \Gamma(k) \equiv -Re[z_\pm(k)]/k^2. \]

In classical hydrodynamics \((k \to 0)\), the transport coefficients are \(k\)-independent by definition. However, when this situation does not hold, but the hydrodynamic modes are still clearly separated from the kinetic modes, one can speak of a \textit{generalized hydrodynamic} regime \([\text{9}]\), with transport coefficients which are slowly varying functions of \(k\). In lattice-based models, the transport coefficients might also depend on the direction of the wave vector, \(\hat{k}\), reflecting anisotropies due to the symmetry of the lattice. By computing the transport coefficients through the spectral analysis of the evolution operator, and looking at their \(k\)-dependence, one can judge the range of validity of the classical and the generalized hydrodynamic regime. In a previous analysis \([\text{9}]\), for the simplest Lattice-gas FHP-I model with a density of \(\rho = 1.8\), generalized hydrodynamics were shown to be valid up to \(k \simeq 0.4\) for certain directions of \(k\) (Figure 3 of reference \([\text{9}]\)).

In order to allow for an analysis of \(H(k)\) for the Lattice BGK model, we require an effective collision matrix. It is easy to verify that, with

\[ \Omega_{\alpha\beta} = -\frac{1}{\tau} \left[ \delta_{\alpha\beta} - \frac{1}{b} - \frac{d}{bc^2} c_\alpha \cdot c_\beta \right], \]

Eq. (1) reduces to Eq. (2), conservation of both mass and momentum is satisfied and all the non-zero eigenvalues of \(\Omega\) are equal to \(-1/\tau\). This matrix can therefore be employed for the analysis.

Figure 1(a) shows the real part of a typical spectrum obtained for the two-dimensional BGK model on a hexagonal lattice with \(\tau = 3/4\) and \(k\) along the \(\hat{x}\) direction (parallel to a lattice vector). One can distinguish the hydrodynamic (shear and sound) as well as the kinetic modes \((Re[z_\lambda(0)] = \ln |1 - 1/\tau|)\). Mixing of the two kinds of modes happens at \(k \simeq 3.0\). Figure 1(b) displays \(-Re[z_\lambda(k)]/k^2\) for the hydrodynamic modes of the same model, and from this figure we conclude that classical hydrodynamics is valid up to \(k \simeq 1.2\) and generalized hydrodynamics up to \(k \simeq 2.1\). This conclusion is supported by Figure 1(c) displaying \(c_s(k) = \pm Im[z_\lambda(k)]/k\). With \(k\) along the \(\hat{y}\)-direction, the ranges are 1.5 and 2.3 respectively. We have studied the same model for values of \(\tau\) ranging from 0.55 to 1.5, and find that the range of classical and generalized hydrodynamics, given by the behaviour of the real and imaginary parts of \(z_\lambda(k)\), is essentially the same.
as for the example given above (i.e. for $\tau = 0.75$) as long as $\tau \leq 1$. For $\tau > 1$, the range rapidly decreases so that, for instance, at $\tau = 4/3$, classical hydrodynamics is only valid up to $k \simeq 0.3$, and generalized hydrodynamics up to $k \simeq 1.3$, for $k$ along the $\hat{x}$-direction.

Since the two-dimensional LBE model allows for an adjustment of two independent parameters, one might expect a greater scope for tuning the behaviour of $z_\lambda(k)$. However, although the quadratic behaviour of $-Re[z_\lambda(k)]$ for hydrodynamic modes can extend over a greater range, we find that correspondingly, linear behaviour of $Im[z_\lambda(k)]$ is found over a smaller range: the overall range of validity of generalized hydrodynamics is scarcely improved compared to the Lattice BGK model. Our “optimum range” is very comparable with that for multispeed FHP Lattice-gas models [9], where the best results were obtained for the 7-bit FHP-III model.

Analysis for the four-dimensional LBE and Lattice BGK models based on the FCHC lattice proceeds similarly. Two and three dimensional data can be obtained from these four dimensional models by projecting the lattice onto two or three dimensions and defining a reduced collision matrix [2]. Our numerical studies show that the spectral behaviour of $H(k)$ constructed with the full matrix or the reduced matrices is identical, at least for the physically important hydrodynamic modes. We therefore present results only for the full four-dimensional FCHC lattice.

For the BGK model, we have again used values of $\tau$ ranging from 0.55 to 1.5. Our findings are that classical hydrodynamics is valid up to $k \simeq 1.0$ and generalized hydrodynamics up to $k \simeq 2.0$, independent of $\tau$, as long as $\tau \leq 1$. As in two dimensions, the ranges rapidly decrease for $\tau > 1$, with, at $\tau = 4/3$, classical hydrodynamics being only valid up to $k \simeq 0.3$, and generalized hydrodynamics up to $k \simeq 1.3$. These ranges, although smaller or comparable to those for the two-dimensional models based on the hexagonal lattice, are still considerable: they suggest that generalized hydrodynamics is valid down to a spatial scale of around three lattice spacings.

The four dimensional LBE model allows for an adjustment of three independent parameters. As in the two-dimensional case, the range of validity of generalized hydrodynamics is hardly changed compared to the Lattice BGK model, but the quadratic behaviour of $-Re[z_\lambda(k)]$ for the hydrodynamic modes can be
tuned and extended up to $k \simeq 1.5$ (for example with $\lambda = -3/2$, $\sigma = \gamma = -1$ as in Fig.2). In general terms, this seems to correspond to the existence of kinetic modes which, at $k=0$, are less clearly separated from the hydrodynamic regime.

We thus conclude that the computational advantages of the Lattice BGK algorithm are complemented by a significant range of validity for classical and generalized hydrodynamics. In two dimensions, using a single speed model on a hexagonal lattice, the range is as good as that for LGA models. For two- and three-dimensional models based on the FCHC lattice, the range is as good or better than that for more general LBE methods. The additional parameters available in the LBE method seem to give no further advantage. We expect that future applications of the Lattice BGK algorithm will exploit this situation.

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References

[1] U. Frisch, D. d’Humières, B. Hasslacher, P. Lallemand, Y. Pomeau and J.-P. Rivet, Complex Syst. 1, 649 (1987) [reprinted in *Lattice Gas Methods for Partial Differential Equations*, edited by G. Doolen (Addison-Wesley, Singapore, 1990)]

[2] R. Benzi, S. Succi and M. Vergassola, Phys. Rep. 222 147 (1993)

[3] S. Chen, Z. Wang, X. Shan and G. D. Doolen, J. Stat. Phys 68 379 (1992)

[4] Y.H. Qian, D. d’Humières and P. Lallemand, Europhys. Lett. 17 479 (1992)

[5] A.K. Gunstensen, D.H. Rothman, S. Zaleski and G. Zanetti, Phys. Rev A 48 4320 (1991)

[6] A.J.C. Ladd, Phys. Rev. Lett. 70 1339 (1993)

[7] L.-S. Luo, H. Chen, S. Chen, G.D. Doolen and Y.-C. Lee, Phys. Rev. A 43 7097 (1991)

[8] P. Grosfils, J.-P. Boon, R. Brito and M.H. Ernst, to appear in Phys. Rev. E

[9] S.P. Das, H.J. Bussemaker and M.H. Ernst, Phys. Rev. E 48 245 (1993)

[10] D. d’Humières and P. Lallemand, Complex Syst. 1 599 (1987)

[11] F.J. Higuera, S. Succi and R. Benzi, Europhys. Lett. 9 345 (1989)

[12] P. Bhatnagar, E.P. Gross and M.K. Krook, Phys. Rev. 94 511 (1954)
Captions

FIG. 1. (a) Real part of the spectrum for the two-dimensional BGK model with \( \tau = 3/4 \) and \( k \parallel \hat{x} \). The upper of the two hydrodynamic modes \((-Re[z_\lambda(k)] \sim O(k^2) \text{ as } k \to 0)\) is the diffusive shear mode \((\lambda = \perp)\), while the lower curve corresponds to the propagating sound modes \((\lambda = \pm)\). (b) The corresponding plot of \(-Re[z_\lambda(k)]/k^2\) for the hydrodynamic modes. The upper curve corresponds to the kinematic viscosity \(\nu(k)\), while the lower curve is the sound damping constant \(\Gamma(k)\). (c) The sound velocity \(c_s(k) = \pm Im[z_\pm(k)]/k\) for the same model.

FIG. 2. (a) Viscosity \(\nu(k)\) (upper continuous curve) and sound damping constant \(\Gamma(k)\) (lower continuous curve) for a four-dimensional LBE model, with \(\lambda = -3/2, \sigma = \gamma = -1\) and \(k \parallel \hat{x}\). The dashed lines correspond to kinetic modes. (b) The sound velocity \(c_s(k) = \pm Im[z_\pm(k)]/k\) for the same model.
