Progress in the Understanding of the Fluctuating Lattice Boltzmann Equation

Burkhard Dünweg[a], Ulf D. Schiller[a], Anthony J. C. Ladd[b]

[a] *Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany*
[b] *Chemical Engineering Dept., University of Florida, Gainesville, FL 32611-6005, USA*

Abstract

We give a brief account of the development of methods to include thermal fluctuations into lattice Boltzmann algorithms. Emphasis is put on our recent work (Phys. Rev. E 76, 036704 (2007)) which provides a clear understanding in terms of statistical mechanics.

Key words:
Lattice Boltzmann, thermal fluctuations, Langevin equation, Monte Carlo, detailed balance
PACS: 47.11.Qr, 47.57.-s

The lattice Boltzmann (LB) equation has, in the last few decades, emerged as a powerful tool to solve fluid dynamics problems numerically [1, 2]. The algorithm is a fully discretized version of the Boltzmann equation, known from the kinetic theory of gases. Space $\vec{r}$ is discretized in terms of a regular (usually simple-cubic) lattice with spacing b, time t in terms of a time step h, and velocity space in terms of a small set of velocities $\vec{c}_i$ that are chosen such that $\vec{c}_i h$ is a vector which connects two nearby lattice sites. For example, the popular D3Q19 model [3] employs nineteen velocities, corresponding to zero and the six nearest and twelve next-nearest neighbors on a simple-cubic lattice. The central quantities on which the algorithm operates are the populations $n_i(\vec{r},t)$, representing the mass density corresponding to velocity $\vec{c}_i$, such that the total mass density $\rho(\vec{r},t)$ at the site $\vec{r}$ at time t is given by

$$\rho(\vec{r},t) = \sum_i n_i(\vec{r},t). \tag{1}$$

Similarly, the momentum density is obtained as the first velocity moment,

$$\vec{j}(\vec{r},t) = \sum_i n_i(\vec{r},t)\vec{c}_i, \tag{2}$$

and the hydrodynamic flow velocity is given by

$$\vec{u}(\vec{r},t) = \frac{\vec{j}(\vec{r},t)}{\rho(\vec{r},t)}. \tag{3}$$

The algorithm is then described by the lattice Boltzmann equation

$$n_i(\vec{r}+\vec{c}_i h, t+h) = n_i^\star(\vec{r},t) = n_i(\vec{r},t) + \Delta_i\left(\{n_i(\vec{r},t)\}\right). \tag{4}$$

The collision operator Δ_i modifies the populations on the site ($\{n_i\}$ denotes the set of all populations on the site), such that mass and momentum are conserved. Energy conservation is not taken into account, since we are here interested in an isothermal version, where the temperature instead of the energy is fixed (formally, this corresponds to a system with infinite heat conductivity). The conservation equations therefore read

$$\sum_i \Delta_i = \sum_i \Delta_i \vec{c}_i = 0. \tag{5}$$

This results in a set of post-collisional populations $n_i^\star$, which are then propagated to the neighboring sites.

In most applications, it is assumed that Δ_i is a deterministic variable, i. e. that it can be calculated in a unique fashion from the populations $n_i(\vec{r},t)$. This is very much in spirit of the original continuum Boltzmann equation, and applicable to many practical problems of fluid flow. However, for soft-matter applications, where one is interested in Brownian motion of suspended particles, or similar phenomena, this is not sufficient. Rather, one must take into account that here both the lattice spacing b and the time step h are so small that on these scales thermal fluctuations are sizeable and cannot be viewed as just averaged out. Indeed, assuming that the underlying physical model is an ideal gas, one can see this rather easily by starting from the equation of state

$$k_B T = m_p c_s^2, \tag{6}$$

where k_B is Boltzmann's constant, T is the absolute temperature, m_p is the mass of a gas particle, and c_s is the isothermal speed of sound ($c_s^2 =$

p/ρ, where p is the thermodynamic pressure). Usually, c_s is chosen as an adjustable parameter, picked in such a way that — even in nonequilibrium situations like shear flow — the typical flow velocity u is small compared to c_s. This is the condition of low Mach number flow, which is needed because of the restricted velocity space (note that c_s is of the order of the c_i). Furthermore, the physics of the problem usually dictates the values of k_BT and ρ — for example, we may assume that we study water at room temperature. Equation 6 then allows us to determine the mass of a gas particle, m_p, which, in turn, determines the number of particles on a lattice site (assuming a simple-cubic lattice in three dimensions),

$$N_p = \frac{\rho b^3}{m_p}. \tag{7}$$

If this number is very large, fluctuations will strongly average out, i. e. one can consider the single lattice site as a thermodynamic system. This is the case for typical engineering applications. However, if N_p is comparable to unity, as it is the case for many soft-matter applications, then fluctuations are important, and must be taken into account in the algorithm. Since the system is an ideal gas, N_p is a random variable whose probability distribution is Poisson. For such a distribution, the variance is identical to the mean, i. e. the relative importance of fluctuations is given by

$$Bo = \frac{\left(\left\langle N_p^2\right\rangle - \left\langle N_p\right\rangle^2\right)^{1/2}}{\left\langle N_p\right\rangle} = \left\langle N_p\right\rangle^{-1/2} = \left(\frac{m_p}{\rho b^3}\right)^{1/2} = \left(\frac{k_BT}{\rho b^3 c_s^2}\right)^{1/2} \tag{8}$$

(we coined the word "Boltzmann number" for this parameter). We thus see that the degree of fluctuations is controlled by the degree of coarse-graining, through the lattice spacing b. It is also useful to introduce the parameter

$$\mu = \frac{m_p}{b^3} = \frac{k_BT}{b^3 c_s^2}, \tag{9}$$

which may be called the thermal mass density.

The question of how to actually implement these fluctuations in the collision operator Δ_i has found different answers during the last fifteen years, with increasing level of refinement and understanding. In what follows, we wish to briefly outline these developments. Since all the material has been published previously, we would like to be brief, and refer the interested reader

to the original papers [4, 5, 6, 7] as well as to a recent review [8], in which all the technical details have been worked out and explained in depth.

The first implementation of a fluctuating lattice Boltzmann equation was by Ladd [4, 5]. He started from the well-understood deterministic version ($Bo = 0$), and added a stochastic term Δ_i' to the collision operator, with the requirement that this is consistent, on the macroscopic scale, with fluctuating hydrodynamics, as given by Landau and Lifshitz [9].

Let us first discuss the deterministic version in some more detail. It is based upon a linearized collision operator,

$$\Delta_i = \sum_j L_{ij}(n_j - n_j^{eq}), \tag{10}$$

where the matrix L_{ij} contains constant elements, and is implicitly given via a diagonal representation (see below), while n_i^{eq} is the lattice analog to a velocity-dependent Maxwell-Boltzmann distribution:

$$n_i^{eq}(\rho, \vec{u}) = a^{c_i}\rho\left(1 + \frac{\vec{u}\cdot\vec{c}_i}{c_s^2} + \frac{(\vec{u}\cdot\vec{c}_i)^2}{2c_s^4} - \frac{u^2}{2c_s^2}\right). \tag{11}$$

Here c_s is the speed of sound, and the weights $a^{c_i} > 0$ are normalized such that $\sum_i a^{c_i} = 1$. This notation has been chosen in order to emphasize that, for symmetry reasons, the weights only depend on the absolute values of the speeds c_i, but not on their direction. Furthermore, the weights are adjusted in such a way that n_i^{eq} satisfies the properties

$$\sum_i n_i^{eq} = \rho, \tag{12}$$

$$\sum_i n_i^{eq}\vec{c}_i = \vec{j}, \tag{13}$$

$$\sum_i n_i^{eq}\vec{c}_i \otimes \vec{c}_i = \rho c_s^2 \overleftrightarrow{1} + \rho\vec{u}\otimes\vec{u} = \overleftrightarrow{\Pi}^{eq}. \tag{14}$$

For D3Q19, this implies $a^{c_i} = 1/3$ for the rest population, $a^{c_i} = 1/18$ for the nearest neighbors, and $a^{c_i} = 1/36$ for the next-nearest neighbors. Furthermore $c_s^2 = (1/3)(b^2/h^2)$.

L_{ij} is implemented as follows: First, one transforms to so-called "modes", i. e. linear combinations of the n_i which are adapted to the symmetry of the problem. The first ten modes have a direct hydrodynamic interpretation:

- Mode 0: Mass density $\rho = \sum_i n_i$.
- Modes 1-3: Momentum density $j_\alpha = \sum_i n_i c_{i\alpha}$; here α denotes a Cartesian index.
- Modes 4-9: Stresses $\Pi_{\alpha\beta} = \sum_i n_i c_{i\alpha} c_{i\beta}$, which are conveniently decomposed into trace and traceless part: $\Pi_{\alpha\beta} = \bar{\Pi}_{\alpha\beta} + \frac{1}{3}\delta_{\alpha\beta}\Pi_{\gamma\gamma}$; here we use the Einstein summation convention.

The additional modes (so-called "kinetic" or "ghost" modes) do not have a direct relation to hydrodynamics. In the D3Q19 model, there are nine such modes, which are explicitly listed in Ref. [8]. After having calculated the (pre-collisional) modes, one leaves the conserved modes unchanged, while the other modes are linearly relaxed towards their local equilibrium value. The stresses are changed from pre- to post-collisional values according to

$$\begin{aligned} \bar{\Pi}^{\star\, neq}_{\alpha\beta} &= \gamma_s \bar{\Pi}^{neq}_{\alpha\beta}, \\ \Pi^{\star\, neq}_{\alpha\alpha} &= \gamma_b \Pi^{neq}_{\alpha\alpha}, \end{aligned} \tag{15}$$

where we use the notation $n_i^{neq} = n_i - n_i^{eq}$. The kinetic modes are defined in such a way that their equilibrium part is zero, and the action of L_{ij} on them is, in the simplest version, just a projection, such that the post-collisional kinetic modes vanish.

A Chapman-Enskog analysis shows that this procedure yields the Navier-Stokes equations of hydrodynamics in the limit of large length and time scales, with shear and bulk viscosities that are uniquely determined by the values of γ_s and γ_b, respectively. Linear stability requires $|\gamma_s| < 1$, $|\gamma_b| < 1$, corresponding to positive values of the viscosities.

This deterministic procedure was modified by Ladd [4, 5] by just changing Eq. 15 to

$$\begin{aligned} \bar{\Pi}^{\star\, neq}_{\alpha\beta} &= \gamma_s \bar{\Pi}^{neq}_{\alpha\beta} + \bar{R}_{\alpha\beta}, \\ \Pi^{\star\, neq}_{\alpha\alpha} &= \gamma_b \Pi^{neq}_{\alpha\alpha} + R_{\alpha\alpha}, \end{aligned} \tag{16}$$

with suitably chosen random stresses $R_{\alpha\beta}$, while the treatment of the kinetic modes was left unchanged. The rationale behind this procedure was that the kinetic modes do not contribute to hydrodynamics, and the goal was to simulate the fluctuations correctly on the hydrodynamic scale. On this

scale, however, the fluctuating stresses $\hat{R}_{\alpha\beta}$ that appear in the Navier-Stokes equation (different from $R_{\alpha\beta}$ that appears in Eq. 16) satisfy the relations [9]

$$\begin{aligned} \left\langle \hat{R}_{\alpha\beta} \right\rangle &= 0, \qquad (17) \\ \left\langle \hat{R}_{\alpha\beta}\left(\vec{r},t\right) \hat{R}_{\gamma\delta}\left(\vec{r}',t'\right) \right\rangle &= 2k_B T \eta_{\alpha\beta\gamma\delta}\, \delta\left(\vec{r}-\vec{r}'\right) \delta\left(t-t'\right) \\ &\rightarrow \frac{2k_B T}{b^3 h} \eta_{\alpha\beta\gamma\delta}\, \delta_{\vec{r}\vec{r}'} \delta_{tt'}, \end{aligned}$$

where $\eta_{\alpha\beta\gamma\delta}$ is the isotropic fourth-rank viscosity tensor, parameterized by shear and bulk viscosity, or the relaxation parameters γ_s and γ_b. In the last step, we have discretized the delta functions by the lattice parameter b and the time step h, as it is appropriate for a lattice simulation.

One might expect that the LB noises are just given by $R_{\alpha\beta} = \hat{R}_{\alpha\beta}$. However, this turns out not to be correct [4, 5]. Rather, the correct fluctuating LB stresses are obtained by a suitable modification of the amplitude. For the shear stresses one has, for example,

$$\left\langle R_{xy}^2 \right\rangle = \left(1-\gamma_s\right)^2 \left\langle \hat{R}_{xy}^2 \right\rangle. \qquad (18)$$

The same modification factor occurs for all other shear stresses, too, while the corresponding factor for the bulk stresses is $(1-\gamma_b)^2$. The reason has been explained in detail in Refs. [4, 5]; essentially the renormalization of the amplitude comes from the fact that Eq. 17 describes the physics on a more coarse-grained time scale than Eq. 16 — the delta correlation in time is in LB replaced by an exponential decay. However, the time integral of the correlation functions must be the same in order to obtain the same macroscopic viscosities.

Adhikari et al. [6] then generalized this procedure by not only thermalizing the stresses, but also the kinetic modes, which were treated in a rather similar fashion to Eq. 16. The argument was that the relaxation of kinetic modes introduces an additional dissipative mechanism into the system, which should be balanced by a compensating Langevin noise. A projection should be viewed as the limit of such a relaxation, with relaxation parameter $\gamma \rightarrow 0$, such that the fluctuation-dissipation relation should hold in this case, too. While this argument makes intuitive sense, and led to a substantially improved representation of the fluctuations at short length scales [6], the theoretical foundation of this procedure remained somewhat obscure (at least to the present authors).

In a recent publication [7] we have been able to resolve these questions by developing a first-principles theory of thermal fluctuations in LB models. The starting point was the observation that for a discrete system the concept of a fluctuation-dissipation theorem should rather be replaced by the concept of detailed balance as it applies to Monte Carlo simulations [10]. In order to be able to check whether an update rule satisfies or violates the detailed-balance condition, we therefore explicitly constructed the probability density for the random variables n_i on a site in thermal equilibrium. Taking advantage of the underlying picture of a gas of particles, we first transform from the n_i to variables ν_i, the number of particles on the site which have velocity $\vec{c}_i$ (cf. Eqs. 7 and 9):

$$\nu_i = \frac{n_i}{\mu}. \tag{19}$$

In terms of these variables, the probability density (except for normalization, which is unimportant for our purposes) is written as

$$P\left(\{\nu_i\}\right) \propto \left(\prod_i \frac{\bar{\nu}_i^{\nu_i}}{\nu_i!} \exp\left(-\bar{\nu}_i\right)\right) \delta\left(\sum_i \mu\nu_i - \rho\right) \delta\left(\sum_i \mu\vec{c}_i\nu_i - \vec{j}\right). \tag{20}$$

The underlying picture is that of a "velocity bin" i in thermal contact with a huge reservoir of particles, resulting in a Poisson distribution of the variable ν_i. This distribution is characterized by its mean value $\bar{\nu}_i$, which, for reasons of consistency with the deterministic version, should be proportional to the weight a^{c_i} (see Eq. 11). Normalization requires

$$\bar{\nu}_i = \frac{a^{c_i}\rho}{\mu}. \tag{21}$$

Equation 20 then results from assuming that all the velocity bins on the site are statistically independent, except for the constraints of conserved mass and momentum, which are taken into account by the delta functions, in close analogy to the statistical description of the microcanonical ensemble [11].

The further development is somewhat technical but straightforward and shall be sketched only briefly. We use Stirling's formula and transform back to the n_i to write the factor in front of the delta functions as $\exp(S)$, where the entropy S has a Boltzmann-like form. Maximizing P is equivalent to maximizing S under the constraints of given values for ρ and $\vec{j}$, and the

solution of this problem, up to second order in u, is just Eq. 11, as is well-known from previous studies of the "entropic lattice Boltzmann" approach [12]. Fluctuations around the most probable populations are described by n_i^{neq}, which, within a saddle-point approximation, obey a Gaussian distribution, whose variance is, within a $u \to 0$ approximation, given by $\mu\rho a^{c_i}$. Normalizing the fluctuations to unit variance, followed by an orthonormal transformation to normalized modes $\hat{m}_k^{neq}$, yields a very simple form for the probability distribution,

$$P\left(\{\hat{m_k}^{neq}\}\right) \propto \exp\left(-\frac{1}{2}\sum_{k>3}\hat{m}_k^{neq\,2}\right), \tag{22}$$

where modes $i = 0, \ldots, 3$ do not occur due to mass and momentum conservation. These modes are updated according to the rule

$$\hat{m}_k^{\star neq} = \gamma_k \hat{m}_k^{neq} + \varphi_k r_k, \tag{23}$$

with adjustable parameters γ_k, φ_k, and normalized, independent Gaussian random numbers r_k. It is then straightforward to show [7, 8] that detailed balance holds exactly for

$$\varphi_k = \left(1 - \gamma_k^2\right)^{1/2}, \tag{24}$$

which turns out to be identical to the prescription of Adhikari et al. [6]. This shows that the stochastic analog of projecting out the kinetic modes is to sample them from scratch, and explains the non-trivial prefactor in the fluctuating stresses in a straightforward way. Furthermore [7, 8], one may apply the Chapman-Enskog procedure to the stochastic version of the algorithm. This shows in a particularly concise way that the behavior in the hydrodynamic limit is given by Landau-Lifshitz fluctuating hydrodynamics [9], and that the details of the dynamics of the kinetic modes are indeed immaterial for the behavior in that limit, as already anticipated in Refs. [4, 5]. For practical simulations, however, one should prefer the more recent version which does satisfy detailed balance on the local scale as well. We believe that this is really an improvement that outweighs the computational costs, which are unfortunately not completely negligible. While simple LB algorithms have so few operations per collision step that they are typically limited by the bandwith of memory access in the streaming step [13], this does not seem to be true here, where the generation of random numbers

L	stresses–only	full thermalization
10	0.74	0.47
20	0.66	0.44
30	0.52	0.39

Table 1: Performance of the stochastic D3Q19 algorithm, using an implementation on a 64-bit AMD Athlon 3500+ processor with 2.2 GHz CPU speed and 512 kB cache size. The program is part of the Mainz ESPResSo [14] package. Simulations were run on simple-cubic lattices of size L^3 for 10^5 lattice sweeps, and Gaussian random numbers were generated by the Box-Muller [15] method. Performance data are given in MLUPS (million lattice-site updates per second).

combined with the linear transformation to mode space and back contributes noticeably. In practice, one may say that the additional thermalization of the kinetic modes will slow down the algorithm by roughly $20\% \ldots 40\%$ — at least this is what we observed for our D3Q19 implementation, see Table 1. For large lattices the memory bottlenecks become more important than for small ones; for this reason, the simulations become systematically slower, while the performance difference between "stresses-only" vs. full thermalization becomes less pronounced.

So far, only the case of an isothermal ideal gas has been thoroughly understood. For the future, it is hoped that the present theoretical approach will also help develop an improved understanding of systems with non-trivial equations of state, and systems where thermal conduction and energy conservation are taken into account.

References

[1] Succi, S., *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond*, Oxford University Press, Oxford, 2001.

[2] Benzi, R., Succi, S., and Vergassola, M., Phys. Rep. **222** (1992) 145.

[3] Qian, Y. H., D'Humieres, D., and Lallemand, P., Europhys. Lett. **17** (1992) 479.

[4] Ladd, A. J. C., J. Fluid Mech. **271** (1994) 285.

[5] Ladd, A. J. C., J. Fluid Mech. **271** (1994) 311.

[6] Adhikari, R., Stratford, K., Cates, M. E., and Wagner, A. J., Europhys. Lett. **71** (2005) 473.

[7] Dünweg, B., Schiller, U. D., and Ladd, A. J. C., Phys. Rev. E **76** (2007) 036704.

[8] Dünweg, B. and Ladd, A. J. C., Adv. Polym. Sci. **221** (2009) 89.

[9] Landau, L. D. and Lifshitz, E. M., *Fluid Mechanics*, Addison-Wesley, Reading, 1959.

[10] Landau, D. P. and Binder, K., *A Guide to Monte Carlo Simulations in Statistical Physics*, Cambridge University Press, Cambridge, 2000.

[11] Landau, L. D. and Lifshitz, E. M., *Statistical Physics*, Addison-Wesley, Reading, 1969.

[12] Karlin, I. V., Ferrante, A., and Öttinger, H. C., Europhys. Lett. **47** (1999) 182.

[13] Wellein, G., Zeiser, T., Hager, G., and Donath, S., Computers & Fluids **35** (2006) 910.

[14] Limbach, H.-J., Arnold, A., Mann, B. A., and Holm, C., Comput. Phys. Commun. **174** (2006) 704.

[15] Press, W. H., Flannery, B. P., Teukolsky, S. A., and Vetterling, W. T., *Numerical Recipes*, Cambridge University Press, Cambridge, 1986.