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Cross Correlators and Galilean Invariance in Fluctuating Ideal Gas Lattice Boltzmann Simulations

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Abstract. We analyze the Lattice Boltzmann method for the simulation of fluctuating hydrodynamics by Adhikari et al. [Europhys. Lett., 71 (2005), 473-479] and find that it shows excellent agreement with theory even for small wavelengths as long as a stationary system is considered. This is in contrast to other finite difference and older lattice Boltzmann implementations that show convergence only in the limit of large wavelengths. In particular cross correlators vanish to less than 0.5%. For larger mean velocities, however, Galilean invariance violations manifest themselves.

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Key words: Lattice Boltzmann, fluctuations, Galilean invariance.

1 Introduction

Fluctuations are important for many hydrodynamic phenomena, from colloid diffusion to phase-separation close to the critical point. Particle based methods such as Stochastic Rotation Dynamics [2], Lattice Gas [3] or Molecular Dynamics simulations [4] naturally give rise to stochastic noise. In contrast the lattice Boltzmann (LB), or finite difference discretization of the Navier-Stokes equations require fluctuations that have to be included manually. The guiding principle for doing this is the theory of the fluctuating Navier-Stokes equations [5]. Despite the success of applying the Navier-Stokes equations to very small-scale flows formally the hydrodynamic limit requires large wavelengths. For fluctuating hydrodynamics the constraint of large wavelengths becomes important and standard discretization will give results that are not in agreement with statistical physics for shorter wavelengths. For a detailed analysis of simulating fluctuating hydrodynamics using finite difference methods and some remedies to improve this situation see the recent manuscript of A. Donev [6]. Similar deficiencies are found for implementations of

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fluctuating Navier-Stokes equations using the Lattice Boltzmann approach introduced by Ladd [7]. It is, however possible to use a more fundamental approach to include fluctuations in the LB method. Adhikari et al. [1] introduced noise on all nonconserved modes, not only the hydrodynamic ones, leading to a scheme which shows good agreement with theory even for large wavelengths. Duenweg et al. rederived this noise implementation from detailed balance considerations of lattice gases [8]. Both approaches are numerically identical. In this paper we study the degree of improvement achieved and show that many of the deficiencies that plague finite difference discretizations of fluctuating Navier-Stokes equations are absent in this Lattice Boltzmann implementation as long as we consider a system with vanishing mean velocity. For large mean velocities Galilean invariance is violated and errors of a similar magnitude to the earlier implementations are observed.

2 Fluctuating lattice Boltzmann with ghost noise

Following the derivation of Adhikari et al. [1], we start with the Lattice Boltzmann equation (LBE)

$$f_i(\mathbf{x}+\mathbf{v}_i,t+1)=f_i(\mathbf{x},t)+\sum_j \Lambda_{ij}\Big[f_j(\mathbf{x},t)-f_j^0(\mathbf{x},t)\Big]+\xi_i(\mathbf{x},t). \tag{2.1}$$

Here the f_i are the particle densities at position x, time t associated with velocity $\mathbf{v}_i$. Λ_{ij} is the collision matrix and ξ_i are the noise terms. We use the standard local equilibrium distribution given by

$$f_i^0=\rho w_i\Big[1+\frac{3}{c^2}\mathbf{u}\cdot\mathbf{v}_i+\frac{9}{2c^4}(\mathbf{u}\cdot\mathbf{v}_i)^2-\frac{3}{2c^2}\mathbf{u}\cdot\mathbf{u}\Big], \tag{2.2}$$

which is the discretized version of a Maxwell distribution [9, 10]. In equilibrium the f_i will fluctuate around this distribution. The noise terms ξ_i must be chosen such that, in the case of isothermal Lattice Boltzmann (LB), the density $\rho=\sum_i f_i$ and momentum $\rho\mathbf{u}=\sum_i f_i\mathbf{v}_i$ are conserved, i.e., $\sum_i \xi_i=0$ and $\sum_i \xi_i v_i=0$. Furthermore a proper fluctuation dissipation theorem (FDT) corresponding to the collision operator Λ_{ij} is obeyed. This implies that the ξ_i are correlated. We can find a representation in which the noise terms are uncorrelated by transforming the LBE into moment space. The moments are given by

$$M^a(\mathbf{x},t)=\sum_i m_i^a f_i(\mathbf{x},t). \tag{2.3}$$

So far this is a standard Multi-Relaxation-Time (MRT) representation [11–13]. The back transform is given by $f_i(\mathbf{x},t)=\sum_a n_i^a M^a(\mathbf{x},t)$. However, in order to construct a proper FDT these transforms cannot be orthogonal as in other MRT methods [11,12], so here we have $n_i^a \neq m_i^a$. Instead the transforms are chosen such that

$$\sum_i w_i m_i^a m_i^b=\sum_i m_i^a n_i^b=\delta^{ab} \tag{2.4}$$