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Derivation of Hydrodynamics for Multi-Relaxation Time Lattice Boltzmann using the Moment Approach

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Abstract. A general analysis of the hydrodynamic limit of multi-relaxation time lattice Boltzmann models is presented. We examine multi-relaxation time BGK collision operators that are constructed similarly to those for the MRT case, however, without explicitly moving into a moment space representation. The corresponding 'moments' are derived as left eigenvectors of said collision operator in velocity space. Consequently we can, in a representation independent of the chosen base velocity set, generate the conservation equations. We find a significant degree of freedom in the choice of the collision matrix and the associated basis which leaves the collision operator invariant. We explain why MRT implementations in the literature reproduce identical hydrodynamics despite being based on different orthogonalization relations. More importantly, however, we outline a minimal set of requirements on the moment base necessary to maintain the validity of the hydrodynamic equations. This is particularly useful in the context of position and time-dependent moments such as those used in the context of peculiar velocities and some implementations of fluctuations in a lattice-Boltzmann simulation.

AMS subject classifications: 76P05, 82B40

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1 Introduction

The lattice Boltzmann (LB) method is continuing to increase in popularity as a simulation method for fluid mechanics for a wide range of applications from turbulence [1] to complex fluids [2]. A key of its success is the simplicity of the algorithm. Instead of discretizing the hydrodynamic equations directly the method is based on an underlying microscopic model. Historically the method developed from lattice gases [3] where particles move on a lattice and collide on lattice points. Because such a lattice gas model

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locally conserves mass and momentum the macroscopic behavior of the system has to be described by the continuity and Navier-Stokes equations [4]. The connections between the microscopic streaming and collision rules and the macroscopic differential equations is established by taking the hydrodynamic limit which requires averaging the locally conserved quantities. This reproduces the Boltzmann equation [5]. Performing a Taylor expansion on the discrete Boltzmann equation then leads to a PDE representation of the discrete evolution equation [6].

At this point there are several routes to proceed. Grad [7] suggests taking moments of the full Boltzmann equation which is a route that has been taken by other groups [8]. Alternatively one can formally expand the distribution function before taking the moments, which is known as the Chapman-Enskog expansion [9]. The maximum entropy method is another viable alternative [10]. In the case of convective scaling either approach will lead to identical results to second order: the continuity and Navier-Stokes equations as well as the heat equation for thermal systems. The higher order equations are, however, quite different. Here neither approach has been particularly successful as the Navier-Stokes level equations appear to be appropriate to length-scales close to molecular scale [11]. There are few attempts to derive higher order hydrodynamic equations in the LB context. One recent publication succeeded in deriving third order hydrodynamics with an off-lattice approach [12]. Another exception are multi-phase fluids where higher order spatial derivatives giving rise to surface tension have to be taken into account [13].

The development of the method took a major leap when it was discovered that it is feasible to use a Boltzmann-level microscopic model [14, 15], which removes microscopic noise. This approach is referred to as the lattice Boltzmann method. Higuera and Jiminez already introduced the predecessor of what would become the multi-relaxation time (MRT) technique. Qian *et al.* [16] found that the approach is simplified considerably when the collision operator is written as a single-time BGK expression which relaxes local particle distributions towards the equilibrium distribution. To this date this represents the most popular flavor of lattice Boltzmann algorithms employed.

Shortly after the introduction of the single-time relaxation collision operator d'Humieres reemphasized that one can extend the BGK collision with a multi-relaxation time (MRT) approach [17]. In the MRT description the collision is described with a matrix, which allows for a decoupled relaxation of the different stress terms. It thus decouples the different transport coefficients and they no longer need to take their ideal gas values as in the single time BGK case.

Deriving hydrodynamic equations for multi-relaxation time lattice Boltzmann methods is usually achieved by Chapman-Enskog like expansions. These expansions often depend on the specific model [9]. A good review on lattice Boltzmann was published recently by Dünweg and Ladd [18]. Similar in spirit to the work presented here they attempt to derive the isothermal Navier-Stokes equations in a model independent fashion. In particular they list a set of general conditions that are required to retain hydrodynamics [Eqs. (80–84) in [18]]. However, they state that the details of the implementation of