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Extended BGK Boltzmann for Dense Gases

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Abstract. An alternate BGK type formulation of the Enskog equation has been recently proposed [1]. It was shown that the new model has a valid H-theorem and correct thermal conductivity. We propose Lattice Boltzmann (LB) formulation of this new Enskog-BGK model. The molecular nature of the model is verified in case of shear flow by comparing the predicted normal stress behavior by the current model with the prediction of molecular dynamics simulations. We extend the model for multiphase flow by incorporating attractive part as Vlasov type force. To validate multiphase formulation, the results of 3D simulations of a condensing bubble in a periodic box are presented.

AMS subject classifications: 76T10, 82C40

Key words: Lattice Boltzmann method, multiphase flow, Enskog equation.

1 Introduction

The Lattice Boltzmann Method (LBM) has emerged as an viable alternative to more mature methods such as Discrete simulation Monte Carlo (DSMC) for studying rarefied gas flow in the regime of moderate to low Knudsen number $(\mathrm{Kn} < 1)$ and low Mach number limits $(\mathrm{Ma} \ll 1)$ [2–8]. Apart from efficient discretization, the important feature which makes the method very efficient is the use of simplified collision mechanism known as the Bhatnagar-Gross-Krook (BGK) collision approximation [9–12]. While BGK-LBM is an excellent tool for studying dilute gases even at the molecular level [2], the success of the method for dense gas is at best very modest. While a top-down connection from continuum formulation of multiphase flow via diffuse interface theory is on firm ground [13, 14], despite good progress made in connecting these models with Enskog-Vlasov type theories [15–17], so far connection from microscopic theory is not so well settled. Perhaps one of the reason for this is formulating a consistent BGK type model

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for Enskog equation is non-trivial. There is no straightforward extension of BGK for dense gases or multiphase flows, as the equilibrium is still Maxwell-Boltzmann in velocity space but there is a non-ideal contribution to pressure.

The dense gas analog to the Boltzmann equation was given by Enskog [18] who introduced a short range pair correlation function in the collision integral. While the Enskog equation has a valid H-theorem, it is not convenient for simple numerical implementation. Therefore, a BGK type phenomenological model for dense gases can be very useful for simulation of multiphase flows. There have been several attempts to address this issues by expanding the Enskog collision integral around BGK collision term by a formal Hermite expansion [19–21]. The coefficients are then tuned to obtain correct conservation laws. While most of the present Multiphase LBM are based on this class of models, the lack of H-theorem and incorrect thermal conductivity behavior are some of the weakness of these approaches [13, 15, 17, 21, 22]. Recently, some of these issues were resolved in a BGK type formulation for the dense gas [1]. In the present work, we consider this recently proposed extension to the Boltzmann equation, wherein the effect of finite density is accounted at a mean field level by suitable generalization of the advection velocity, while retaining the point-particle based collision integral of the Boltzmann equation. This model has both correct conservation laws as well as a valid H-theorem [1].

We explain the physical motivation of the model and conservation laws in Section 2. In Section 3, we compare the analytical solution of the present model in uniform shear flow (USF) with Molecular Dynamics (MD) to validate its molecular nature. We introduce the model in a discrete velocity lattice in Section 4, following which we extend it to multiphase flows by addition of attractive term in Section 5. We introduce the LB scheme with space and time discretization and discuss the various approximations that are essential to retain the numerical efficiency of BGK-LBM in Section 6. We present results from 1D simulation, including comparison with Maxwell construction in Section 7. Section 8 deals with extension to 3D and results of simulations of a condensing bubble in D3Q27 are presented.

2 Present model

In this section, we will review main features of the modified BGK type of approach for Enskog dynamics as presented in [1]. As compared to Enskog, this model takes an alternate approach to account for the effect of finite density by the generalization of the advection velocity. The physical motivation behind the modification of the advection velocity as opposed to collision is that the effect of the collective motion on the tagged particles will manifest itself as a modification of mean-free path concept. Thus, in this model the evolution equation for the one particle distribution function $f(\mathbf{x},\mathbf{v},t)$ with BGK collision model is given as

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial x_\alpha}(\hat{v}_\alpha f)+\frac{F_\alpha}{m}\frac{\partial f}{\partial v_\alpha}=\frac{f^{\rm eq}-f}{\tau}, \tag{2.1}$$