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A Novel Construction of Distribution Function through Second-Order Polynomial Approximation in Terms of Particle Mass, Momentum and Energy

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Abstract. In this paper, we propose a new way to construct the distribution function through the second-order polynomial approximation in terms of particle mass, momentum and energy. The new construction holds three distinguished features. First, the formulations are more concise as compared with the third-order truncated Hermite polynomial expansion which yields Grad's 13-moment distribution function; Second, all moments of the present distribution function are determined from conservation laws; Third, these moments are closely linked to the most desirable variables, such as mass, momentum and energy. Then, this new distribution function is applied to construct a new gas kinetic flux solver. Numerical validations show that the proposed method recovers the Navier-Stokes solutions in the continuum regime. In addition, it outperforms Grad's 13-moment distribution function in the transition regime, especially in the prediction of temperature and heat flux.

AMS subject classifications: 82C40

Key words: Second-order truncated expansion, peculiar velocity space, compatibility conditions and moment relationships, gas kinetic flux solver, continuum regime to rarefied regime.

1 Introduction

The classical Navier-Stokes (NS) equations have been widely utilized for the research of fluid mechanics. NS equations rely on the assumption of local thermodynamic equi-

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librium. However, this assumption is unjustifiable for systems beyond the continuum flow regime. For example, in the micromachining and micro-electromechanical system (MEMS), the micro-devices are usually in the scale of micrometers. Hence, the characteristic length is usually comparable with the molecular mean free path. In such scenario, the interactions between the molecules are insufficient and the assumption of thermodynamic equilibrium fails, so do the Navier-Stokes (NS) equations established on this assumption.

To describe the non-equilibrium processes, much attention has been put on more sophisticated models, such as kinetic theory and molecular dynamics, which are not constrained by the assumption of thermodynamic equilibrium. The Boltzmann equation is derived from the kinetic theory and physically interprets the collision and transport processes of gas molecules. Based on that, many numerical approaches have been proposed to solve the Boltzmann equation for academic explorations and engineering applications, among which one popular numerical method is the discrete velocity method (DVM). Various versions of DVM include gas kinetic unified algorithm [1, 2], unified gas kinetic scheme [3,4], discrete unified gas kinetic scheme [5,6] and so on. The essence of DVM is to evolve the distribution function of gas molecules, based on which the macroscopic flow variables can be calculated from the moments of the distribution function. However, the evolution of the gas distribution function calls for additional discretization in the particle velocity space, which consumes huge computational efforts and virtual memories.

To avoid the discretization in the velocity space, the explicit formulation of gas distribution function should be given. One common way to construct the gas distribution function is the first-order Chapman-Enskog (CE) expansion [7–11]. Some well-known solvers were proposed based on the CE expansion, such as lattice Boltzmann flux solver (LBFS) [12, 13], gas kinetic scheme (GKS) [14, 15], circular function-based gas kinetic scheme (C-GKS) [16,17], novel gas kinetic flux solver (N-GKFS) [18] and so on. However, the first-order CE expansion can only recover the Navier-Stokes (NS) equations, which constrains the applications of the aforementioned solvers to continuum flow regime at the thermodynamic equilibrium state. To solve flow problems beyond the NS level, a more general distribution function should be adopted. It is noteworthy that the second-order and the third-order CE expansions respectively yield the Burnett and the Supper-Burnett equations. To certain extent, the gas kinetic flux solvers based on these expansions can simulate flows beyond the NS level. However, the gas distribution function that satisfies the Burnett or the Supper-Burnett equations contains the second-order or the third-order spatial derivatives. The treatments of these high-order spatial derivatives complicate the solvers. To alleviate this issue, a variant of gas kinetic flux solver [19] was proposed, which includes the correction terms to the linearized constitutive relations and Fourier's law. The validation results showed that the correction terms indeed take effect in the non-equilibrium regime. However, the effectiveness of the correction terms will reduce with the increasing of the Knudsen numbers.

Another way to construct the gas distribution function is the Hermite polynomial expansion [20]. The regularized 13-moment method [21] and regularized 26-moment