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Construction of Non-Equilibrium Gas Distribution Functions through Expansions in Peculiar Velocity Space

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Abstract. Gas distribution function plays a crucial role in the description of gas flows at the mesoscopic scale. In the presence of non-equilibrium flow, the distribution function loses its rotational symmetricity, making the mathematical derivation difficult. From both the Chapman-Enskog expansion and the Hermite polynomial expansion (Grad's method), we observe that the non-equilibrium effect is closely related to the peculiar velocity space (C). Based on this recognition, we propose a new methodology to construct the non-equilibrium distribution function from the perspective of polynomial expansion in the peculiar velocity space of molecules. The coefficients involved in the non-equilibrium distribution function can be exactly determined by the compatibility conditions and the moment relationships. This new framework allows constructing non-equilibrium distribution functions at any order of truncation, and the ones at the third and the fourth order have been presented in this paper for illustration purposes. Numerical validations demonstrate that the new method is more accurate than the Grad's method at the same truncation error for describing non-equilibrium effects. Two-dimensional benchmark tests are performed to shed light on the applicability of the new method to practical engineering problems.

AMS subject classifications: 76P05
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1 Introduction

The gas distribution function is a probability function to describe the molecular behaviors in the phase velocity space. It plays essential roles in modeling gas flows from the

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mesoscopic perspective in a way that the moments of the gas distribution function recover macroscopic flow variables such as density, velocity and temperature. In equilibrium state, the gas distribution function can be exactly derived as the Maxwellian distribution [1]. This distribution function is unimodal with Gaussian-like forms and possesses rotational symmetricity in the phase velocity space [2]. However, in the presence of non-equilibrium flows (e.g., the shock wave structure [3–5], asymmetric features such as bimodal forms arise in the distribution function, which increment the difficulties in constructing mathematical models.

Existing methods to approximate the distribution function for non-equilibrium flows stem from two ideas: the Chapman-Enskog (CE) expansion [6] and the Hermite polynomial expansion [7]. Specifically, the CE expansion performs power series expansion on the equilibrium distribution function [8–10]. With more expansion terms, the constructed distribution function is expected to more precisely describe the deviation from equilibrium state. However, since it is expanded with respect to a term proportional to the Knudsen number [11], this approach naturally fails in recovering strong non-equilibrium behaviors. To alleviate these limitations, Grad [12] approximated the non-equilibrium distribution function in terms of Hermite polynomial expansion. Among various versions of Grad's models, the Grad's 13 distribution function [12] truncating at the third-order Hermite polynomial expansion is perhaps the most classical one, whose capability is mainly recognized in the slip regime and the transition regime at moderate Knudsen number [13]. Stronger non-equilibrium behaviors can be recovered by using the fourth-order Hermite polynomial expansion, which results in Grad's 26 distribution function [14]. However, the Grad's distribution function is derived from the orthogonal Hermite polynomial expansion. As a result, it merely considers the contracted coefficients and contracted polynomials, which strictly satisfy orthogonality. The non-orthogonal terms are never considered and will lose some physical information to some extent.

Hence, it is still desirable to propose an effective distribution function, which could be more capable for the prediction of its shape in the non-equilibrium flows than the one derived from the CE expansion or Hermite polynomial expansion. Existing works show that the non-equilibrium distribution functions derived from CE expansion and Hermite polynomial expansion can be both formulated as an equilibrium distribution function multiplying a revision term ϕ. For the CE expansion method, the term ϕ^{CE} is associated with the gradients of thermodynamic variables and the peculiar velocities [15]. In the meantime, for the Grad's distribution function, the revision term ϕ^{Grad} is mainly made of the high-order moments and the peculiar velocities. Both perspectives imply that the non-equilibrium effect could be closely associated with the peculiar velocities, which leads to a natural question of whether the direct expansion in the peculiar velocity space could construct more accurate non-equilibrium terms. The answer towards this question motivates the present paper.

In this paper, we propose a generalized methodology to construct non-equilibrium gas distribution functions based on the complete polynomial expansion in the peculiar