

Implicit Discrete Unified Gas Kinetic Scheme for Steady Flows of Binary Gas Mixtures

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Abstract. An implicit discrete unified gas kinetic scheme (DUGKS) is developed for multiscale steady flows of binary gas mixtures by solving the Andries-Aoki-Perthame kinetic model (AAP). To ensure the high convergence efficiency for all flow regimes, the microscopic and macroscopic asynchronous iterative strategies are used, where both the macroscopic and microscopic equations are solved iteratively by the Lower-Upper Symmetric Gauss-Seidel (LU-SGS) method. The macroscopic iteration is conducted to solve the macroscopic governing equations containing source terms as an implicit prediction step to evaluate the local equilibrium state of the microscopic evolution, and the macroscopic flux used in the macroscopic iteration is obtained by taking moments of the distribution function. Besides, to keep the asymptotic preserving properties, the numerical flux across the cell interface is reconstructed by the characteristic solution of the kinetic governing equations for both species like the explicit DUGKS for a single gas. Several numerical tests, including the Couette flow, the lid-driven cavity flow, and the flows through a slit of different mixtures, are simulated to verify the accuracy and efficiency of the present scheme for binary mixtures. Furthermore, compared to the explicit DUGKS, the implicit scheme improves the computational efficiency by 1-2 orders of magnitude.

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1 Introduction

Steady rarefied gas mixture flows are ubiquitous in many engineering fields, such as the high-altitude flights, molecular beam technology, vacuum sciences, and so on. Generally, the degree of non-equilibrium of the rarefied flows can be described by the Knudsen number (Kn), which is defined as the ratio of the molecular mean free path (MFP, λ) to the system characteristic length (L), i.e., $Kn = \lambda/L$. For flows in the rarefied regime ($Kn > 0.01$), the macroscopic fluid equations including the Navier-Stokes (NS) and Fourier heat conduction equations fail to capture the non-equilibrium effects. The Boltzmann equation for gas mixtures provides an alternative way to describe flows in the whole regimes from the perspective of kinetic theory [1, 2].

The direct simulation Monte Carlo (DSMC) method [3] is a commonly used stochastic method for solving the Boltzmann equation of high-speed rarefied flows [4, 5], but it is inefficient for near-continuum flows. Besides, the deterministic discrete velocity method (DVM) [6–11] is popular for solving the kinetic model equations. However, the discretization of the kinetic models in the physical and velocity spaces brings in enormous computational burden for three-dimensional (3D) and highly non-equilibrium flows, which is also the common problem undergone by other deterministic methods.

Efforts have been devoted to improving the efficiency of DVM for steady flows by introducing the implicit treatment. Yang and Huang [7] proposed the implicit DVM, where the loss term in the relaxation-type collision term was treated implicitly, while the gain term, i.e., the equilibrium state, was approximated explicitly. Significant efficiency improvement can be observed in the rarefied regime using the implicit DVM, but it is inefficient for flows in the near-continuum regime due to the explicit treatment of the equilibrium state. Similar approaches were proposed [12–14] and slow convergence appeared in the steady computations due to the semi-implicit treatment of the collision term. Subsequently, a fully implicit scheme was developed by Miessens [8, 15, 16] to remedy the deficiency. In this method, the gain term was treated implicitly and predicted by the linear approximation of the loss term. As a result, a fast convergence can be achieved for the steady flows in the near-continuum regime with large time steps. However, a large linear system with a huge Jacobian matrix should be solved in each iteration step. The complexity and huge computational costs make the linear implicit DVM inefficient for 3D and highly non-equilibrium problems. Except the fully implicit scheme, another strategy to accelerate the implicit DVM is the synthetic scheme [17, 18], where the macroscopic moment equations have been introduced and solved iteratively coupled with the kinetic transport equation to significantly accelerate the slow convergence rate of the kinetic transport [19, 20].