A Gas Kinetic Scheme for the Simulation of Compressible Multicomponent Flows

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Abstract. In this paper, a gas kinetic scheme for the compressible multicomponent flows is presented by making use of two-species BGK model in [A. D. Kotelnikov and D. C. Montgomery, A Kinetic Method for Computing Inhomogeneous Fluid Behavior, J. Comput. Phys. 134 (1997) 364-388]. Different from the conventional BGK model, the collisions between different species are taken into consideration. Based on the Chapman-Enskog expansion, the corresponding macroscopic equations are derived from this two-species model. Because of the relaxation terms in the governing equations, the method of operator splitting is applied. In the hyperbolic part, the integral solutions of the BGK equations are used to construct the numerical fluxes at the cell interface in the framework of finite volume method. Numerical tests are presented in this paper to validate the current approach for the compressible multicomponent flows. The theoretical analysis on the spurious oscillations at the interface is also presented.

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Key words: Multicomponent flows, two-species BGK model, Chapman-Enskog expansion, gas kinetic scheme.

1 Introduction

The numerical methods for the compressible multicomponent flows have become important topics in the research of computational fluid dynamics. Over the past decades,

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significant progresses have been made to handle the multicomponent flows which are associated with discontinuities and shock waves. One of the popular approaches is to solve an extended system in which additional conservation equations are introduced to the original Euler equations. The additional equations describe the conservation of parameters, such as level set functions, mass fraction and ratio of specific heats in the mixture [1, 6, 13, 16, 21]. In order to eliminate the spurious oscillations and other computational inaccuracies in the conservative methods [1, 2, 11], some non-conservative approaches which capture the contact discontinuous by making use of additional non-conservative governing equations were proposed [1, 2, 11, 18–20, 22]. Another approach introduced by Karni [12] was to solve the Euler equations separately on each side of the interface by a method designed for a single-component flow, while the interface was dealt with in a different manner using a pressure evolution equation derived from the energy equation. Despite the fact that the method is not exactly conservative at the interface, reasonable results can be also obtained.

In recent years, the gas kinetic scheme based on the BGK model [3-5] for the compressible fluids proposed in [24,25] has attracted much attention. Based on the Chapman-Enskog expansion, the Euler as well as Navier-Stokes equations can be derived from the gas kinetic BGK model. In the framework of finite volume method, the BGK scheme makes use of the local integral solution of BGK model to compute a time-dependent gas distribution function at a cell interface. The numerical fluxes are obtained by taking moments of the distribution function in the gas evolution stage. As the BGK model is a statistical model, the particle transports and collisions are coupled in the whole gas evolution process, and the particle collision time controls the physical dissipative coefficients in the macroscopic equations. Since the gas evolution is associated with a relaxation process, i.e. from a non-equilibrium state to an equilibrium one, the entropy condition is satisfied automatically. Once the physical structure can be well resolved by the numerical cell size, in smooth regions, the scheme automatically gives an accurate compressible Navier-Stokes solution. Meanwhile, in the discontinuous regions, because of the delicate dissipative mechanism, the BGK scheme generates a stable and crisp shock transition. The BGK scheme has been extended to magnetohydrodynamics [23,28], hyperbolic conservation laws with source terms [24] and shallow water flow [30]. The high order BGK scheme has also been developed [14,27]. Recently, a unified gas kinetic scheme [29] is developed for all Knudsen number flows, which is an extension of the gas-kinetic scheme from the continuum flow to the rarefied regime with discretization of velocity space.

The BGK-Based numerical methods for the multicomponent flow have also been proposed in recent years. A gas kinetic scheme for multicomponent flow was presented in [15, 26]. The basic idea of this method is that the evolution of each component is governed by a BGK model with its own equilibrium state, and the equilibrium states of both components are coupled in space and time due to the course of particle collisions, and the common variables in the equilibrium states are the macroscopic velocities and temperatures. By incorporating a conservative γ -model proposed in [1] into the BGK scheme, a gas kinetic γ -model BGK scheme for the compressible multicomponent flow