Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2017-0023

Vol. **22**, No. 4, pp. 1123-1149
October 2017

A Two-Stage Fourth-Order Gas-Kinetic Scheme for Compressible Multicomponent Flows

Liang Pan[1,*], Junxia Cheng[1], Shuanghu Wang[1] and Kun Xu[2]

[1] *Institute of Applied Physics and Computational Mathematics, Beijing, China.*
[2] *Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*

Received 24 January 2017; Accepted (in revised version) 22 March 2017

Abstract. With the use of temporal derivative of flux function, a two-stage temporal discretization has been recently proposed in the design of fourth-order schemes based on the generalized Riemann problem (GRP) [21] and gas-kinetic scheme (GKS) [28]. In this paper, the fourth-order gas-kinetic scheme will be extended to solve the compressible multicomponent flow equations, where the two-stage temporal discretization and fifth-order WENO reconstruction will be used in the construction of the scheme. Based on the simplified two-species BGK model [41], the coupled Euler equations for individual species will be solved. Each component has its individual gas distribution function and the equilibrium states for each component are coupled by the physical requirements of total momentum and energy conservation in particle collisions. The second-order flux function is used to achieve the fourth-order temporal accuracy, and the robustness is as good as the second-order schemes. At the same time, the source terms, such as the gravitational force and the chemical reaction, will be explicitly included in the two-stage temporal discretization through their temporal derivatives. Many numerical tests from the shock-bubble interaction to ZND detonative waves are presented to validate the current approach.

AMS subject classifications: 76T10, 76P05, 76N15

Key words: Multicomponent flows, gas kinetic scheme, two-stage temporal discretization.

1 Introduction

The development of numerical methods for compressible multicomponent flows is important in computational fluid dynamics. Over the past decades, significant progresses have been made for the computations of multicomponent flows which are associated

*Corresponding author. *Email addresses:* panliangjlu@sina.com (L. Pan), cheng_junxia@iapcm.ac.cn (J. X. Cheng), wang_shuanghu@iapcm.ac.cn (S. H. Wang), makxu@ust.hk (K. Xu)

with discontinuities and shock waves. One of the popular approaches is to solve an extended system in which additional equations are introduced to the original Euler equations in order to track different components. The additional equations can be the equations for the volume fraction, mass fraction, and ratio of specific heats of the mixture [1, 6, 35]. In order to eliminate spurious oscillations and other computational inaccuracies in the conservative methods, some non-conservative approaches which capture the contact discontinuities by making use of additional non-conservative governing equations were proposed [1, 2, 17, 27, 36]. Another approach is the sharp interface method. Each fluid is solved separately on each side of the interface by the method designed for a single-component flow. Interfaces between different fluids are captured by the level-set method [30] or front tracking method [38, 39]. Boundary conditions at interface are given by ghost-fluid method or application of exact Riemann solver at the interface [6,39]. Although interface can be resolved sharply, it is difficult to apply these methods to the interfaces associated with complex geometry.

The gas-kinetic scheme has been developed systematically for the compressible flow computations [42,43]. An evolution process from kinetic scale to hydrodynamic scale has been constructed for the flux evaluation. The kinetic effect through particle free transport contributes to the artificial dissipation for the capturing of shock waves, and the hydrodynamic effect plays a dominant role for the capturing of resolved viscous and heat conducting solutions. In this sense, the gas-kinetic scheme is hybrid method of upwind and central difference, but with a smooth transition between these two limits. Due to the coupling of inviscid and viscous terms in the kinetic formulation, there is no fundamental barrier for the finite volume gas-kinetic scheme to capture Navier-Stokes solutions with structured or unstructured meshes. With the discretization in particle velocity space, a unified gas-kinetic scheme has been developed for the transport process in the entire flow regimes from rarefied to continuum ones [11, 26, 44]. Recently, with the incorporation of higher-order initial data reconstruction, a third-order gas-kinetic scheme has been proposed in [22, 25, 29]. The flux evaluation is based on the time evolution solution of flow variables from initial piece-wise discontinuous polynomials around a cell interface. However, based on the time accurate evolution solution from a general initial condition for the flux function, the gas-kinetic scheme becomes complicated for its further improvement of the order of the scheme, such as the construction of a fourth-order flux function [24]. However, instead of developing one step time integration method, the two-stage Lax-Wendroff time stepping method in [21] provides an alternative framework to develop a fourth-order gas-kinetic scheme with a second-order flux function only [28]. In comparison with the formal one-stage time-stepping third-order gas-kinetic solver, the fourth-order method not only reduces the complexity of the flux function, but also improves the accuracy of the scheme, even though the third- and fourth-order schemes have similar computation cost. Most importantly, the robustness of the fourth-order gas-kinetic scheme is as good as the second-order one.

The BGK-based numerical methods for the multicomponent flow have also been proposed in recent years. By incorporating a conservative γ-model [1] into the gas-kinetic