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Implicit unified gas-kinetic scheme for steady state solutions in all flow regimes

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ABSTRACT

This paper presents an implicit unified gas-kinetic scheme (UGKS) for non-equilibrium steady state flow computation. The UGKS is a direct modeling method for flow simulation in all regimes with the updates of both macroscopic flow variables and microscopic gas distribution function. By solving the macroscopic equations implicitly, a predicted equilibrium state can be obtained first through iterations. With the newly predicted equilibrium state, the evolution equation of the gas distribution function and the corresponding collision term can be discretized in a fully implicit way for fast convergence through iterations as well. The lower–upper symmetric Gauss–Seidel (LU-SGS) factorization method is implemented to solve both macroscopic and microscopic equations, which improves the efficiency of the scheme. Since the UGKS is a direct modeling method and its physical solution depends on the mesh resolution and the local time step, a physical time step needs to be fixed before using an implicit iterative technique with a pseudo-time marching step. Therefore, the physical time step in the current implicit scheme is determined by the same way as that in the explicit UGKS for capturing the physical solution in all flow regimes, but the convergence to a steady state speeds up through the adoption of a numerical time step with large CFL number. Many numerical test cases in different flow regimes from low speed to hypersonic ones, such as the Couette flow, cavity flow, and the flow passing over a cylinder, are computed to validate the current implicit method. The overall efficiency of the implicit UGKS can be improved by one or two orders of magnitude in comparison with the explicit one.

1. Introduction

The gas-kinetic scheme (GKS) based on the kinetic model equations, such as the Bhatnagar–Gross–Krook (BGK) model [1] of the Boltzmann equation, was proposed by Prendergast and Xu [2,3] for the Euler and high Reynolds number Navier–Stokes (NS) solutions, which has been further developed by Xu [4] for the accurate capturing of low Reynolds number flows as well. The GKS is a robust and accurate scheme for the NS solutions in the smooth region and provides delicate numerical dissipation through particles transport and ineffective collision for the construction of a non-equilibrium numerical shock structure. Since the GKS updates the macroscopic flow variables only and uses the Chapman–Enskog expansion [5] for

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the construction of a gas distribution function, it is only valid for the continuum flow. In order to extend the scheme for the non-equilibrium flow computation, the gas distribution function itself has to be updated for the capturing of highly non-equilibrium state. With a discretized particle velocity space, a unified gas-kinetic scheme (UGKS) has been constructed for all flow regimes [6,7]. The central ingredient of the UGKS is to use the integral solution of the BGK-type model equation for the gas evolution and the flux evaluation at a cell interface. Due to the multiscale nature of the integral solution, i.e., a time-dependent transition from the kinetic scale particle free transport to the hydrodynamic scale wave propagation, the UGKS can automatically recover flow physics in different regimes with the variation of the ratio between the time step and the local particle collision time. Besides the coupling of particle transport and collision for the gas evolution around a cell interface, this kind of coupling is also necessary for the evaluation of a time-dependent gas distribution function inside each control volume [8]. As a result, the cell size and the time step used in UGKS are not limited by the particle mean free path and mean collision time, and the ratio between the mesh size and particle mean free path can be changed dramatically in different flow regimes. This unified approach provides a promising and general tool for the capturing of multi-scale transport physics, such as rarefied gas dynamics, radiative heat transfer, and plasma evolution [9,10]. In comparison with the direct simulation Monte Carlo (DSMC) method [11] and other discrete velocity methods (DVM) [12–14], the UGKS shows better accuracy and efficiency in the near continuum flow regime. However, in order to make the scheme become a valuable tool in real engineering applications, there is a high demand to develop an implicit UGKS method for fast convergence to the steady state solution, such as in the designs of micro–electro–mechanical system (MEMS) and thermal protection system of spacecrafts. Different from the particle-based DSMC method, there are still discretized governing equations in the UGKS, and the equation-based techniques can be fully utilized for the development of implicit method.

For the GKS, several implicit algorithms have been developed to simulate continuum flow. An early one was based on a simplified gas-kinetic scheme by Chae et al. [15], where alternating direction implicit (ADI) method was applied to solve the implicit equations in multi-dimensional cases. Since the lower–upper symmetric Gauss–Seidel (LU-SGS) factorization method was developed by Yoon and Jameson [16–18], it has been widely used in flow computations [19,20]. The LU-SGS technique has been used in the construction of implicit GKS [21]. Many acceleration techniques, such as local time stepping, multi-grid strategy, and matrix-free LU-SGS iteration have been added into the implicit schemes [22,23]. Moreover, the implicit GKS has also been applied for near continuum flow [22] and with unstructured meshes [24].

For rarefied flow computation, implicit schemes for kinetic model equations with the discretization of gas distribution function can be designed as long as the equilibrium state g^{n+1} in the collision term is known. In Yang and Huang's implicit scheme [25], the equilibrium state g^{n+1} is simply replaced by g^n with an explicit treatment. With a similar treatment, an implicit method for the UGKS has been constructed recently as well [26]. As analyzed by Mieussens [12,13], it may slow down the convergence of an implicit scheme considerably if the gain and loss terms in the kinetic model equations are evaluated at different time levels. The implicit treatment of [26] seems less effective in continuum flow regime and its efficiency may depend sensitively on the numerical tests. Another implicit method for the discrete velocity model is to approximate the equilibrium state g at the next time level [12,13] with a linear mapping between the equilibrium state g and the real gas distribution function f. But, this mapping involves a huge matrix, which increases the complexity of the implicit method. For BGK-type model equation, a moment-based accelerating technique has been developed recently in [27], coupling the kinetic equation and fluid momentum equations.

The present work is to develop an implicit UGKS method, where both macroscopic and microscopic governing equations will be fully coupled in an implicit way. In order to treat the collision term in a fully implicit way, the equilibrium state will be predicted first by solving the macroscopic governing equations implicitly. With the predicted conservative flow variables, the governing equation of the distribution function can be fully discretized implicitly, where a diagonal matrix system about the unknown distribution function will be formed. Then, both matrix systems derived from implicit macroscopic equations and implicit microscopic equation are solved iteratively by using LU-SGS method.

The rest of this paper is organized as follows. In section 2, the explicit UGKS scheme is briefly introduced and the implicit method is presented in details. Section 3 tests the implicit UGKS through the cases of low speed Couette and cavity flows, and high speed flow around a cylinder. The efficiency of the implicit UGKS will be compared with the explicit one and other implicit methods. The last section is the conclusion.

2. Unified gas-kinetic scheme

The UGKS is a direct modeling method for the time evolution of a gas distribution function f in a control volume around space $\vec{x}$, time t, and particle velocity $\vec{u}$,

$$\int_{\Omega} (f(\vec{x},t,\vec{u}) - f_0(\vec{x},\vec{u}))dV + \int_0^t \oint_{\partial\Omega} f\vec{u}\cdot d\vec{S}dt = \int_0^t \int_{\Omega} Q(f,f)dt, \tag{1}$$

where Ω is a control volume in physical space, and $\partial\Omega$ is the boundary of the control volume. The f_0 is the initial gas distribution function at time $t = 0$. Here $Q(f,f)$ is the collision term and its effect on the time evolution of f depends on the scale of t. The governing equations for the macroscopic flow variables are based on the modeling equations as well,