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A semi-implicit gas-kinetic scheme for smooth flows

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ABSTRACT

In this paper, a semi-implicit gas-kinetic scheme (SIGKS) is derived for smooth flows based on the Bhatnagar–Gross–Krook (BGK) equation. As a finite-volume scheme, the evolution of the average flow variables in a control volume is under the Eulerian framework, whereas the construction of the numerical flux across the cell interface comes from the Lagrangian perspective. The adoption of the Lagrangian aspect makes the collision and the transport mechanisms intrinsically coupled together in the flux evaluation. As a result, the time step size is independent of the particle collision time and solely determined by the Courant–Friedrichs–Lewy (CFL) condition. An analysis of the reconstructed distribution function at the cell interface shows that the SIGKS can be viewed as a modified Lax–Wendroff type scheme with an additional term. Furthermore, the addition term coming from the implicitness in the reconstruction is expected to be able to enhance the numerical stability of the scheme. A number of numerical tests of smooth flows with low and moderate Mach numbers are performed to benchmark the SIGKS. The results show that the method has second-order spatial accuracy, and can give accurate numerical solutions in comparison with benchmark results. It is also demonstrated that the numerical stability of the proposed scheme is better than the original GKS for smooth flows.

1. Introduction

In recent years, kinetic methods have drawn particular attention as newly-developing computational fluid dynamics (CFD) technology. Unlike the conventional CFD methods based on direct discretizations of the Navier–Stokes (NS) equations, kinetic methods are based on kinetic theory or microparticle dynamics, which provides theoretical connection between hydrodynamics and the underlying microscopic physics, and thus yields efficient tools for multiscale flows. Up to date, a variety of mesoscopic methods have been proposed, such as the lattice gas cellular automata (LGCA) [1], the lattice Boltzmann equation (LBE) [2,3], the gas-kinetic scheme (GKS) [4–11], and the smoothed particle hydrodynamics (SPH) [12], among which the LBE and GKS are specifically designed for CFD. The kinetic nature of the LBE and GKS has led to many distinctive advantages that distinguish them from the classical CFD methods. Specifically, for the LBE method, the convection operator (or streaming process) in phase space is linear, which is same as the Boltzmann equation and contrasts with the nonlinear convection terms in classical CFD methods [13]; in addition, the pressure in LBE methods is calculated using an equation of the state, whereas in classical CFD methods, a Poisson equation with velocity strains should be solved to get the pressure, which often produces numerical difficulties requiring special treatment, such as iteration or relaxation [13]. Furthermore, the kinetic nature of LBE guarantees the intrinsic parallelism feature of the LBE, which makes it more straightforward than the classical CFD methods to implement the Message Passing Interface (MPI) and Graphics Processing Unit (GPU) to improve the computational efficiency [13]. Different from the LBE methods aiming to solve nearly incompressible flows, the GKS is designed mainly for compressible flows, especially shock problems that involve both discontinuous and continuous regimes, which is the numerical challenge for the classical CFD methods. In GKS, by constructing the interfacial fluxes based on certain kinetic equations, a smooth transition between the upwind and central difference mechanics can be realized, which ensures the capability of the scheme for capturing shock discontinuity and smooth flows simultaneously [14,15]. Particularly, the GKS for the Navier–Stokes solutions has been well developed [4,7,8,16–19], and successfully applied to a variety of flow problems [20–23].

As a kind of finite-volume scheme, the key ingredient in GKS for NS solutions is to construct the flux at the cell interface. With

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different approaches, several kinetic schemes have been developed based on the kinetic theory, such as the Kinetic Flux Vector Splitting (KFVS) [7,8,24] scheme based on the collisionless Boltzmann equation and the GKS based on the Bhatnagar–Gross–Krook (BGK) equation where the particle collisions are considered in the construction of the numerical flux. It is shown that the GKS methods avoid the ambiguity of adding *ad hoc* "collisions" for the KFVS to reduce the numerical dissipations [7,8]. Among the BGK-type schemes, the gas-kinetic BGK scheme for the NS solutions has been well developed [4], and has been successfully applied for the continuum flow simulation from low-speed incompressible to hypersonic compressible flows [16,17,25].

In this paper, we present a semi-implicit gas-kinetic scheme (SIGKS), as an alternative BGK-type scheme for smooth flows. The most distinguished feature of the proposed scheme is that the construction of the flux at the cell interface is based on the discrete characteristic solution of the BGK equation, which comes from the Lagrangian aspect. This approach results in the particle collision and transport mechanisms coupled together within a time step, which makes the new scheme exhibited low numerical dissipation and the time step decoupled from the particle collision time. Furthermore, the flux is evaluated in an implicit manner in the scheme, which is expected to have improved numerical stability in comparison with the original GKS method. A set of numerical simulations are carried out and to verify the present scheme as a feasible NS solver.

The rest of the article is organized as follows. The semi-implicit gas-kinetic scheme is derived in Section 2; analysis of numerical flux error of the SIGKS and comparison with the original GKS are made in Section 3; numerical tests are made in Section 4 to validate the performance of the new scheme, and finally some conclusions are drawn in Section 5.

2. Semi-implicit gas-kinetic scheme

The Boltzmann equation expresses the behavior of a many-particle kinetic system in terms of the evolution equation of the singlet gas distribution function. One of its simplified version is the BGK model [26],

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\nabla f=\Omega\equiv\frac{g-f}{\tau}, \tag{1}$$

where f is the gas distribution function and g is the equilibrium state approached by f. Both f and g are functions of space $\boldsymbol{x}$, time t, particle velocities $\boldsymbol{\xi}$, and internal variable $\boldsymbol{\eta}$. The particle collision time τ is related to the viscosity and the heat conduction coefficients. The equilibrium state is a Maxwellian distribution,

$$g=\frac{\rho}{(2\pi RT)^{(D+K)/2}}\exp\left(-\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2+\boldsymbol{\eta}^2}{2RT}\right) \tag{2}$$

where D is the spatial dimension, K is the internal degree of freedom, ρ is the density, $\boldsymbol{u}$ is the macroscopic velocities, R is the gas constant, and T is the gas temperature. The connection between the distribution function f and conservative variable $\boldsymbol{W}$ is

$$\boldsymbol{W}=\begin{pmatrix}\rho\\ \rho\boldsymbol{u}\\ \rho\epsilon\end{pmatrix}=\int\boldsymbol{\psi}f d\Xi, \tag{3}$$

and the fluxes are computed as

$$\boldsymbol{F}=\begin{pmatrix}F_\rho\\ F_{\rho\boldsymbol{u}}\\ F_{\rho\epsilon}\end{pmatrix}=\int\boldsymbol{\xi}\boldsymbol{\psi}f d\Xi, \tag{4}$$

where $d\Xi=d\boldsymbol{\xi}d\boldsymbol{\eta}$ is the volume element in phase space with $d\boldsymbol{\eta}=d\eta_1 d\eta_2\ldots d\eta_K$, and $\boldsymbol{\psi}$ is given by

$$\boldsymbol{\psi}=[\psi_1,\psi_2,\psi_3]^T=\left[1,\boldsymbol{\xi},\frac{1}{2}\left(\boldsymbol{\xi}^2+\boldsymbol{\eta}^2\right)\right]^T.$$

Since mass, momentum and energy are conserved during particle collisions, f and g satisfy the conservation constraint

$$\int(g-f)\boldsymbol{\psi}d\Xi=0, \tag{5}$$

at any point in space and time.

In order to develop a finite volume scheme, the computational domain is first divided into a set of control volumes. Then, we multiply $\boldsymbol{\psi}$ on both sides of Eq. (1), and integrate it in phase space and physical space over a control volume V_i from t_n to t_{n+1}, due to the conservation of conservative variables during particle collision process, the update of the conservative variables at the center of the V_i becomes

$$\boldsymbol{W}_i^{n+1}=\boldsymbol{W}_i^{n}-\frac{\Delta t}{|V_i|}\boldsymbol{F}^{n+1/2}, \tag{6}$$

where

$$\boldsymbol{F}^{n+1/2}=\int\int_{\partial V_i}(\boldsymbol{\xi}\cdot\boldsymbol{n})\,\boldsymbol{\psi}f\,(\boldsymbol{x},\boldsymbol{\xi},t_n+h)\,d\boldsymbol{S}d\Xi \tag{7}$$

is the macroscopic flux across the cell interface and $h=\Delta t/2$. The mid-point rule is employed in the time domain integration of the convection term.

The key ingredient in updating the averaged conservative variables according to Eq. (6) is to evaluate the flux $\boldsymbol{F}^{n+1/2}$, which can be solely determined by the gas distribution function $f\,(\boldsymbol{x},\boldsymbol{\xi},t_n+h)$. Here the Lagrangian perspective is applied in the construction of $f\,(\boldsymbol{x},\boldsymbol{\xi},t_n+h)$: we integrate Eq. (1) within a half time step along the characteristic line with the end point $(\boldsymbol{x}_b)$ located at the cell interface, and use the trapezoidal rule to evaluate the collision term,

$$\begin{aligned}&f\,(\boldsymbol{x}_b,\boldsymbol{\xi},t_n+h)-f\,(\boldsymbol{x}_b-\boldsymbol{\xi}h,\boldsymbol{\xi},t_n)\\&=\frac{h}{2}\left[\Omega(\boldsymbol{x}_b-\boldsymbol{\xi}h,\boldsymbol{\xi},t_n)+\Omega(\boldsymbol{x}_b,\boldsymbol{\xi},t_n+h)\right].\end{aligned} \tag{8}$$

Approximating $f\,(\boldsymbol{x}_b-\boldsymbol{\xi}h,\boldsymbol{\xi},t_n)$ and $g(\boldsymbol{x}_b-\boldsymbol{\xi}h,\boldsymbol{\xi},t_n)$ by their Taylor expansions around $\boldsymbol{x}_b$, we can rewrite Eq. (8) that

$$\begin{aligned}f\,(\boldsymbol{x}_b,\boldsymbol{\xi},t_n+h)=&f\,(\boldsymbol{x}_b,\boldsymbol{\xi},t_n)-h\boldsymbol{\xi}\cdot\nabla f\,(\boldsymbol{x}_b,\boldsymbol{\xi},t_n)\\&+\frac{h}{2}\left[\Omega(\boldsymbol{x}_b,\boldsymbol{\xi},t_n)-h\boldsymbol{\xi}\cdot\nabla\Omega(\boldsymbol{x}_b,\boldsymbol{\xi},t_n)\right.\\&\left.+\Omega(\boldsymbol{x}_b,\boldsymbol{\xi},t_n+h)\right]+O(h^2).\end{aligned} \tag{9}$$

Since the present scheme is targeting the numerical NS solutions in a resolved dissipative region, the Chapman–Enskog expansion can be employed to approximate the distribution function. Then, two approximations can be applied to Eq. (9). First, f is approximated by its first-order Chapman–Enskog expansion, $f\approx g-\tau(g_t+\boldsymbol{\xi}\cdot\nabla g)$, and the second approximation is that $\nabla f\approx\nabla g$, which is consistent with the first-order Chapman–Enskog expansion and includes only the first-order derivatives of the hydrodynamic variables ρ, $\boldsymbol{u}$, and T. Up to this point, the distribution function at the cell interface can be approximated as

$$\begin{aligned}f(\boldsymbol{x}_b,t_n+h)=&\left(\frac{2\tau}{2\tau+h}-\frac{2\tau-h}{2\tau+h}\tau A-\tau\boldsymbol{\xi}\cdot\boldsymbol{a}\right)g(\boldsymbol{x}_b,t_n)\\&+\frac{h}{2\tau+h}g(\boldsymbol{x}_b,t_n+h),\end{aligned} \tag{10}$$

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