Computers and Fluids 127 (2016) 211–225

Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/compfluid

Discrete unified gas kinetic scheme on unstructured meshes

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ARTICLE INFO

Article history:
Received 15 September 2015
Revised 4 January 2016
Accepted 11 January 2016
Available online 14 January 2016

Keywords:
Kinetic equation
Unstructured mesh
Shakhov model

ABSTRACT

The recently proposed discrete unified gas kinetic scheme (DUGKS) is a finite volume method for multiscale flow computations with asymptotic preserving property. The solution of the Boltzmann model equation is directly used for the construction of numerical flux and makes the scheme applicable in all flow regimes. In previous applications of the DUGKS, structured meshes have been mostly employed, which may have difficulties for problems with complex geometries. In this paper we will extend the DUGKS to unstructured meshes, with the implementation of computational fluid dynamics techniques to the DUGKS. Several test cases, i.e., the cavity flow ranging from continuum to free molecular regimes, a multiscale flow problem between two connected cavities with large pressure and density variations, high speed flows past multiple cylinders in slip and transitional regimes, and an impulsive start problem are performed. The results are compared with the well-defined Direct Simulation Monte Carlo (DSMC) or Navier–Stokes (NS) solutions in their applicable regimes. The numerical results demonstrate the effectiveness of the proposed DUGKS for the study of multiscale flow problems.

1. Introduction

Gas flows can be classified into different flow regimes based on the Knudsen number (Kn), which is defined as the ratio of the mean free path of the gas to the physical characteristic length. For flow with Kn $>$ 0.001, non-equilibrium effects become important and the classical Navier–Stokes–Fourier (NSF) equations fail to describe such a flow [1], while the Boltzmann equation can serve as a fundamental equation which is valid in the whole range of Knudsen numbers.

There are mainly two types of numerical approaches to solve the Boltzmann equation. The first one is the widely used direct simulation Monte Carlo (DSMC) method [1], which is the prevailing technique for simulating high-speed rarefied gas flows. However, the DSMC is a single scale method, where the particle transport and collision processes are decoupled. As a result, the cell size and time step are required to be smaller than the mean free path and the mean particle collision time [1]. For flows in near continuum or continuum regime, this requirement will lead to enormous computational costs. Another undesired feature of the DSMC is the statistical noise that must be reduced through intensive sampling and averaging, which is more serious for low speed and small temperature variation flows [1]. Great efforts have been devoted to reduce statistical noise of the DSMC method [2,3]. The second approach for solving the Boltzmann equation is to use deterministic numerical schemes, i.e., the Discrete Velocity Methods (DVM) [4–6]. Most DVM schemes are single scale methods with decoupled particle transport and collision, which have the same constraints on the time step and cell size as the DSMC [7–9]. Recently, some asymptotic preserving (AP) schemes have been proposed to overcome these disadvantages (e.g., [10–12]). The AP schemes for Boltzmann equation are designed to reduce to the appropriate discretization schemes for hydrodynamic equations automatically as the Knudsen number goes to zero, without resolving the mean free path and particle collision time on the computational grids. The AP schemes also treats the collision term implicitly using efficient manners to overcome the stiffness problem as the Knudsen number approaches to zero. Their stability is independent of the Knudsen number. These schemes are able to recover the Euler solutions in the continuum limit, but it is still unclear whether the Navier–Stokes solutions can be accurately obtained [13].

Recently, a unified gas kinetic scheme (UGKS) has been constructed for all Knudsen number flows [14–17]. The UGKS is an aggressive extension of the gas kinetic scheme (GKS) which is a flux solver for hydrodynamic equations and is mainly used to simulate continuum flows [18]. In the UGKS, the particle transport and collision effects are coupled when updating the discrete distribution function. Consequently, the restrictions on the cell size and time

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http://dx.doi.org/10.1016/j.compfluid.2016.01.006
0045-7930/

step are avoided, and the UGKS solutions depend on the ratio of the local time step to the particle collision time [13].

An alternative unified kinetic method, i.e., the discrete unified gas kinetic scheme (DUGKS), has been proposed for multi-regime flow computations recently [19,20]. The DUGKS shares the same modeling mechanism as the UGKS [19]. The main difference between the UGKS and the DUGKS lies in the construction of numerical flux for the discrete distribution function at cell interface. In UGKS, the flux is obtained from the time-dependent distribution function at the cell interface, and this solution is based on the local analytical integral solution of the model kinetic equation. While in DUGKS, the flux is calculated from the distribution function at a half time step, and this solution is determined from a numerical characteristic solution of the model kinetic equation. The flux in DUGKS couples the effects of particle transport and collision, and the updating rule is much simpler than the UGKS.

The DUGKS shares some similarities with the well-known lattice Boltzmann method (LBM) which can be viewed as a special discrete velocity type method. Both of them are based on the relaxation-type collision models, and employ the implicit-to-explicit transformation. The idea behind the flux evaluation method in the DUGKS is conceptually very similar to the streaming step of the LBM, i.e., the particles arrived at the cell face (in the DUGKS) or lattice node (in the LBM) are assumed to have streamed from the upwind, with collision effect considered. However, there are considerable differences between the DUGKS and the LBM. The LBM is essentially an Navier–Stokes equation solver under the low Mach number condition, thus can only be used to simulating near incompressible continuum flows. The DUGKS employing the LBM type discrete velocity set (i.e., the DnQm lattices) can be viewed as a finite-volume based off-lattice Boltzmann method. Their relative performances for continuum flows have been compared in [21]. It is also found that the DUGKS is not a straight forward *translation* of the finite-difference interpreted LBM [22].

In previous works [19,20], the DUGKS has been applied to both low speed and high speed non-equilibrium flows using structured meshes. However, most non-equilibrium flow problems involve complicated geometries, such as those in the microelectromechanical systems (MEMS) industrial and aerospace engineering. The use of unstructured mesh is preferable. In this work we aim to extend the DUGKS to unstructured meshes and demonstrate its effectiveness for the multiscale non-equilibrium flows.

The rest of the paper is organized as following. In Section 2, the general procedure of the DUGKS on unstructured meshes is presented. In Section 3, several numerical examples, including the micro cavity flow, an expansion flow between two connected cavities, and the rarefied gas flow passing through a single and double circular cylinders, will be computed to demonstrate the capability of the current method in simulating flows in different regimes. An additional test case, the impulsive start plate problem is used to verify the uniform convergence rate of DUGKS. A brief summary is given in the last section.

2. Discrete unified gas kinetic scheme

2.1. Shakhov model

The DUGKS is based on the Boltzmann model equation. In this study, the collision operator is approximated by the Shakhov model [23] for monatomic gases. In D dimensional space, the model equation is

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\nabla f=-\frac{1}{\tau}\left[f-f^S\right], \tag{1}$$

where $f=f(\boldsymbol{\xi},\boldsymbol{\eta},\boldsymbol{x},t)$ is the velocity distribution function of particles with velocity $\boldsymbol{\xi}=(\xi_1,\ldots,\xi_D)$ in D dimensional velocity space at position $\boldsymbol{x}=(x_1,\ldots,x_D)$ and time t. Here $\boldsymbol{\eta}=(\xi_{D+1},\ldots,\xi_3)$ is a vector in a space with dimension $L=3-D$, which accounts for the degrees of freedom other than the D-dimensional translational ones. f^S is the Shakhov equilibrium distribution function given by the Maxwellian distribution function f^{eq} plus a heat flux correction term

$$f^S=f^{eq}\left[1+(1-\mathrm{Pr})\frac{\boldsymbol{c}\cdot\boldsymbol{q}}{5pRT}\left(\frac{c^2+\eta^2}{RT}-5\right)\right]=f^{eq}+f_{Pr}, \tag{2}$$

where Pr is the Prandtl number and $\boldsymbol{c}=\boldsymbol{\xi}-\boldsymbol{U}$ is the peculiar velocity around the averaged macroscopic fluid velocity $\boldsymbol{U}$; $\boldsymbol{q}$ is the heat flux, R is the specific gas constant, and T is the temperature. The collision time τ in Eq. (1) is related to the dynamic viscosity μ and pressure p by $\tau=\mu/p$. The dynamic viscosity μ depends on temperature as

$$\mu=\mu_{\mathrm{ref}}\left(\frac{T}{T_{\mathrm{ref}}}\right)^{\omega}, \tag{3}$$

where μ_{ref} is the viscosity at the reference temperature T_{ref}, and the exponent ω is a constant depends on the inter-molecular interaction model. The viscosity μ_{ref} can be related to the reference mean free path λ_{ref}. By using the Knudsen (Kn), Mach (Ma) and Reynolds (Re) numbers, the $\mu_{\mathrm{ref}}\sim\lambda_{\mathrm{ref}}$ relation leads to (Eq. 1.29 in [24]),

$$\mathrm{Kn}=\sqrt{\frac{2\gamma}{\pi}}\frac{(5-2\omega)(7-2\omega)}{15}\frac{\mathrm{Ma}}{\mathrm{Re}}, \tag{4}$$

where γ is the heat capacity ratio. The Kn, Ma and Re numbers are define as

$$\mathrm{Kn}=\frac{\lambda_{\mathrm{ref}}}{L_{\mathrm{ref}}},\quad \mathrm{Ma}=\frac{U_{\mathrm{ref}}}{\sqrt{\gamma RT_{\mathrm{ref}}}},\quad \mathrm{Re}=\frac{\rho_{\mathrm{ref}}U_{\mathrm{ref}}L_{\mathrm{ref}}}{\mu_{\mathrm{ref}}}, \tag{5}$$

where L_{ref}, U_{ref}, ρ_{ref} are the referenced length, velocity and density, respectively.

The Maxwellian distribution function f^{eq} is given by

$$f^{eq}=\frac{\rho}{(2\pi RT)^{3/2}}\exp\left(-\frac{c^2+\eta^2}{2RT}\right), \tag{6}$$

where ρ is the gas density. The conservative flow variables $\boldsymbol{W}\equiv(\rho,\rho\boldsymbol{U},\rho E)^T$ are calculated as moments of the distribution function,

$$\boldsymbol{W}=\int\boldsymbol{\psi}f\mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}, \tag{7}$$

here $\boldsymbol{\psi}=\left(1,\boldsymbol{\xi},\frac{1}{2}(\xi^2+\eta^2)\right)^T$ and $\rho E=\frac{1}{2}\rho U^2+C_VT=\frac{1}{2}\rho U^2+p/(\gamma-1)$, where C_V is the heat capacity. The heat flux $\boldsymbol{q}$ is defined by

$$\boldsymbol{q}=\frac{1}{2}\int\boldsymbol{c}(c^2+\eta^2)f\mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}. \tag{8}$$

The parameter $\boldsymbol{\eta}$ can be viewed as internal degree of freedom, and the dependence of f on $\boldsymbol{\eta}$ can be removed by using two reduced distribution functions [25]

$$g(\boldsymbol{x},\boldsymbol{\xi},t)=\int f(\boldsymbol{\xi},\boldsymbol{\eta},\boldsymbol{x},t)\mathrm{d}\boldsymbol{\eta}, \tag{9a}$$

$$h(\boldsymbol{x},\boldsymbol{\xi},t)=\int\eta^2f(\boldsymbol{\xi},\boldsymbol{\eta},\boldsymbol{x},t)\mathrm{d}\boldsymbol{\eta}. \tag{9b}$$

The conservative macroscopic variables can be computed from these reduced distribution functions as

$$\rho=\int g\mathrm{d}\boldsymbol{\xi},\quad \rho\boldsymbol{U}=\int\boldsymbol{\xi}g\mathrm{d}\boldsymbol{\xi},\quad \rho E=\frac{1}{2}\int(\xi^2g+h)\mathrm{d}\boldsymbol{\xi}, \tag{10}$$

and the heat flux can be computed as

$$\boldsymbol{q}=\frac{1}{2}\int\boldsymbol{c}(c^2g+h)\mathrm{d}\boldsymbol{\xi}. \tag{11}$$