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Improvement of computational efficiency of circular function-based gas kinetic scheme by using Jacobian-free Newton–Krylov method

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ABSTRACT

The gas-kinetic BGK scheme is a promising method for simulation of inviscid and viscous flows. Different from conventional Navier–Stokes (N-S) solvers, it evaluates the inviscid and viscous fluxes simultaneously by reconstructing the local solution of BGK Boltzmann equation at the cell interface. Due to its inherently superior dissipation property, it usually gives accurate and robust numerical results. However, a notable drawback of the BGK-type scheme is the low computational efficiency. Recently, aimed at reducing the computational effort, a circular function-based BGK (CBGK) scheme was developed. Nevertheless, it is still time consuming because the original scheme used an explicit way in the time integration as in most existing BGK schemes and the convergence speed can be slow. To improve the computational efficiency, an implicit CBGK scheme is developed in this paper by incorporating the Jacobian-free Newton–Krylov (JFNK) method into the scheme. Particularly, the generalized minimal residual (GMRES) approach is employed to iteratively solve the large linear equation system. With the help of the Jacobian-free approach, a faster convergence speed can be achieved without explicitly computing and storing the flux Jacobian, which is usually a large and sparse matrix. In order to reduce the number of GMRES iterations, the preconditioning is also adopted and the Lower-Upper symmetric Gauss-Seidel (LUSGS) scheme is employed as a preconditioner. For validation of the present CBGK-JFNK method, several two-dimensional inviscid and viscous test cases are investigated. The numerical results show that the needed computational time is significantly reduced as compared with the original explicit CBGK scheme and the CBGK-LUSGS method.

1. Introduction

In recent decades, the development of numerical schemes based on the gas-kinetic theory has attracted more and more attention [1–10]. Different from conventional Navier–Stokes (N-S) solvers where the inviscid and viscous parts of fluxes at the cell interface are separately computed by different approaches, gas-kinetic schemes evaluate the total fluxes simultaneously by reconstructing the solution of the Boltzmann equation. Physically, it avoids the disparity in N-S solvers that for evaluation of inviscid flux, an assumption of discontinuity is usually made at the cell interface in solving one-dimensional Riemann problem, while for evaluation of viscous flux, the flow is assumed to be smooth across the cell interface in order to obtain the derivatives. Numerically, it is easier to construct multi-dimensional models since the Boltzmann equation is only a scalar equation with the only unknown being the gas distribution function. Also, because the Boltzmann equation has a more fundamental physical basis, gas-kinetic schemes can be suitable for a wide range of flow regimes.

Among all the gas-kinetic schemes, a distinct and attractive one is the BGK scheme, which was first proposed by Prendergast and Xu [3,11]. Compared with some other gas-kinetic schemes such as Equilibrium Flux Method (EFM) [1] and Kinetic Flux Vector Splitting (KFVS) scheme [2] which solve the collisionless Boltzmann equation, the BGK scheme additionally considers the particle collisions in the whole gas evolution process. The collision term is approximated based on the Bhatnagar-Gross-Krook (BGK) model [12]. The inclusion of real collision effect is extremely useful in providing adequate numerical dissipation for invsicid and viscous computations. It has been proven that in smooth regions, the BGK scheme gives accurate N-S solutions, while in the discontinuity regions, it shows a superior dissipation property, which is helpful to capture a crisp and stable shock structure [4,6,13]. Since the entropy condition is intrinsically satisfied, some common numerical difficulties such as “sonic glitch" or “carbuncle phenomenon" are avoided in the BGK scheme. Thus it is free of artificial fixes, which are often needed in conventional schemes for an accurate and robust solution. Some other desirable characteristics of the BGK scheme can be referred to [13].

In spite of these appealing features, a significant drawback which cannot be ignored in the BGK scheme is the low computational efficiency. It is known that the original BGK scheme con-

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sists of many terms and coefficients such as those associated with the approximation of non-equilibrium distribution function, which makes the scheme be relatively complicated. The computational efforts are also usually larger than those of regular N-S solvers. To reduce the computational efforts, several researchers have proposed feasible ways to simplify the original BGK scheme. For example, in the work of Chae et al. [14], the spatial slope term in the equilibrium distribution function is discarded since it is thought to be undesirable for the design of the BGK scheme. The temporal slope term, which provides no help to steady-state calculations, is also neglected. A similar modification was earlier suggested by Xu et al. [4] for inviscid flows, where only the point-wise values are kept in the expansion of gas distribution function and its equilibrium state. Recently, considering that the original Maxwellian function-based BGK schemes involve complicated error and exponential functions, Yang et al. [15] developed a circular function-based BGK (CBGK) scheme for simulation of inviscid flows, where the equilibrium state is represented by a simple circular function. It is shown that the solution accuracy remains comparable to that of the original BGK scheme while the computational cost is effectively reduced. Later, in developing the viscous CBGK scheme, Yang et al. [16] employed a simple way to calculate the non-equilibrium part of the gas distribution function. That is, with the help of Chapman-Enskog (C-E) expansion analysis, the non-equilibrium part can be approximated as the difference of equilibrium distribution function at the cell interface and its surrounding points. Note that this idea was first applied in lattice Boltzmann flux solvers [17]. By adopting the same idea, Sun et al. [18] also developed an efficient gas-kinetic flux solver for both incompressible and compressible viscous flows, where the explicit formulations for computing the numerical fluxes at the cell interface can be simply derived.

Although with these simplification work, the BGK-type scheme may be still time consuming, which cannot be efficiently applied for engineering problems. The reason is that most schemes adopt explicit time integration methods for the update of the solution and the allowable computational time step is thus limited. Moreover, it is well known that the original BGK scheme gives time-dependent flux, therefore the computational time step must be chosen no more than the minimum value among all the local time steps, which further handicaps the convergence of the scheme to a steady state [13]. In this case, to accelerate the computational speed, several implicit BGK schemes have been developed. As shown in the work of Chae et al. [14], the time-averaged flux is first calculated by using a flux averaging time step and then an implicit Alternating Direction Implicit (ADI) scheme [19] is employed for the time integration where a large local time step can be applied. Similarly, with the construction of a time-averaged flux function, Jiang and Qian [20] developed an implicit BGK scheme by adopting the lower-upper symmetric Gauss Seidel (LUSGS) method [21]. The numerical results show a significant acceleration to capture the steady-state solution and a dramatic reduction of the needed CPU time. Some other work to construct LUSGS-based implicit BGK schemes include Xu et al. [7], Li et al. [22], Li and Fu [23] and Zhu et al. [24].

However, as we all know, both ADI and LUSGS schemes treat the BGK scheme-based linear equation system in an approximate way and do not pay off to solve it very accurately [25]. The approximations mainly come from two aspects: one is the factorization error, which is caused by splitting the system matrix into a sum or a product of parts in order to easily obtain the matrix inversion. The other one is associated with the simplification of the flux Jacobian. For example, in the LUSGS scheme, the inviscid flux Jacobian is always computed with a first-order flux-vector splitting approach and the viscous flux Jacobian is approximated by its spectral radii, regardless of the flux solver used for calculation of the residual. This error may become more severe in the BGK scheme since the fluxes in the residual are evaluated from the solution of the BGK Boltzmann equation while the linearization of the residual, i.e., the evaluation of the system matrix, is determined based on the Euler equations. Consequently, these approximations decrease the convergence speed and the maximum time step is possibly limited. Moreover, it has been reported that sometimes the implicit BGK-LUSGS scheme may even suffer a convergence difficulty [7]. To overcome this problem and for further improvement of the computational efficiency, the Jacobian-free Newton–Krylov (JFNK) method is incorporated into the present BGK scheme. Through the use of the JFNK method, the factorization error and the Jacobian simplification-caused error can both be weakened or eliminated. In the Newton–Krylov method, there are usually two levels of iterations. The outer loop is a Newton process for the update of flow solutions. During each outer Newton iteration, the large linear equation system is iteratively solved by the Krylov-subspace methods such as the efficient GMRES method [26]. To avoid explicitly computing and storing the flux Jacobian, the Jacobian-free approach is used, where the product of the flux Jacobian with the solution update is calculated by a simple finite-difference method. This approach also ensures that the system matrix can be evaluated by the BGK scheme, which is used for the residual as well. Due to this consistency, a numerically more accurate linearization of the residual is utilized and thus the quadratic convergence of Newton's scheme can be achieved [25]. Although within this method more computational time may be required for a single time step, the convergence process, however, is greatly accelerated. Practical applications also suggest that the overall time cost can be significantly reduced as compared with the ADI or LUSGS implicit schemes [27–29].

The organization of the paper is as follows: Section 2 is about the construction of the gas-kinetic scheme. Particularly, an efficient CBGK scheme is adopted in this work. Section 3 is about the development of the CBGK-JFNK method and its implementation. Some effective acceleration techniques such as self-adaptive stopping criteria and preconditioning are also demonstrated. Various numerical examples are presented in Section 4. The last section is the conclusion.

2. Circular-function-based gas-kinetic BGK scheme

2.1. Boltzmann equation and circular function

Without consideration of the external forcing term, the BGK Boltzmann equation in a two-dimensional (2D) case can be written as

$$\frac{\partial f}{\partial t}+\xi_x\frac{\partial f}{\partial x}+\xi_y\frac{\partial f}{\partial y}=-\frac{1}{\tau}(f-g) \tag{1}$$

where f is the gas distribution function, g is the equilibrium state approached by f through particle collisions within a relaxation time τ. ξ_x and ξ_y are particle velocities. Since in the BGK scheme, the Boltzmann equation is only locally solved at the cell interface, it is convenient to transform Eq. (1) into a local coordinate system. The x-direction is taken as the normal direction to the local surface and the y-direction is taken as the tangential direction to the local surface.

In the CBGK scheme, based on the assumption that all the particles are concentrated on a circle in terms of mass, momentum and energy conservation, g is represented by a simple circular function. As such, the integral in the infinite domain of phase velocity space is simplified to the line integral along a circle. Because no exponential and error functions are involved in the final formulations for evaluation of the fluxes [15,16], the computational efforts are greatly decreased as compared with the standard BGK scheme. By using the circular function, the equilibrium distribution