

A Hybrid BGK Scheme for Rarefied Gas Flow Computations

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Abstract A hybrid BGK scheme is investigated and developed in this paper. The computational domain is divided into two different types of domains based on the gradient-length based Kn number, and then the direct BGK solver is used to solve the region for the high Kn number region and the BGKX solver is applied to the lower Kn number region. The information between the two flow solver is transferred through ghost cells. The hybrid scheme is applied to the rarefied flow around a cylinder at different Mach numbers. The computational results agrees well with the full direct BGK solver and the computational efficiency has been improved.

INTRODUCTION

Currently there are three categories of solution methods for simulation problems of hypersonic gasdynamics, namely, the continuum CFD, direct simulation Monte Carlo (DSMC) [1] method and the solvers for the Boltzmann equation. Continuum CFD methods could handle amply well these problems insofar as the Kn number be kept small. But the continuum heat flux solution might deteriorate as the flow approaches the transition regime. The DSMC method has the ease of modeling the non-equilibrium physics, yet computationally it becomes increasingly expensive as the Knudsen number approaches the continuum region. The Boltzmann Integro-differential equation (BE) has been in existence since 1872, and the Bhatnagar-Gross-Krook (BGK) model for over 50 years. Many attempts in the past have been directed towards a general numerical method for three dimensional configurations, covering the Knudsen number (Kn) range from continuum, slip, transition to near free molecular flow regimes. Recent achievements among these attempts include solution methods of Lattice Boltzmann Method (LBM) [2], Gaskinetic BGK [3] and Direct Methods [4,5] for solving the Boltzmann Equation, we named direct BE, mostly aimed at general 3D configurations. The latter method solves the complete BE whereas the former two, LBM and Gaskinetic BGK, solve the approximate BGK equation.

Direct BE is to solve the full Boltzmann equation [4-5] with the complete collision integral, which is hampered by the difficulty in coping with the non-equilibrium physics and lacking the macroscopic modeling equations [4]. The computing time for thermal nonequilibrium flow could be comparable if not more expensive than that of DSMC. LBM [2] has been largely confined to low speeds (say, $M < 0.5$). By contrast, the method of gaskinetics BGK by Xu (BGKX method), [3, 6-8] could handle flow regimes including hypersonic flows from continuum to transition with ease of real gas applicability. This method has been successfully applied to simulate many problems in all Mach number ranges, especially on thermal nonequilibrium flows including strong shock waves with some chemical reactions [7,8].

A hybrid method to solve for BE (hybrid BE method, or HBE) has been a continuing R&D subject in recent years, [4, 9]. By hybrid, it means the method combines to solve for the direct BE in the general Kn range with the continuum NS equation in very low Kn range for a "composite" hypersonic rarefied flowfield (hence with a continuum limit). The merit of such an approach is strictly to improve the computational efficiency, as to solve the direct BE would be prohibitively expensive.

In this paper, a hybrid gaskinetic BGK (HBGK) method is developed, which combines to the BGKX equation (for low Kn flow with "composite" hypersonic with a continuum limit), and a direct BGK equation (for higher or general Kn flow) thus yielding a "composite" hypersonic rarefied flowfield. Compared with other hybrid method, the HBGK methods has its own advantages: BGKX scheme is an extension of the gas-kinetic BGK scheme. BGKX is equipped with generalized particle collision time and it is valid even in the transition regime. Therefore, to employ

the relative efficient BGKX will effectively reduce the domain for the direct expensive BGK solver; Direct BGK and BGKX share consistently the same gaskinetic flux through the interface; hence the hybrid gaskinetic BGK (HBGK) renders a consistent numerical approach avoiding flow solution instability.

COMPUTATIONAL METHOD

The BGK and BGKX Equations

For the BGK equation, the right hand side (RHS) of the Boltzmann equation (BE) on the collision terms can be simplified as one relaxation term between equilibrium state, g , and instantaneous distribution, f , while τ is the characteristic relaxation time:

$$\frac{\partial f}{\partial t} + u_i \frac{\partial f}{\partial x_i} = \frac{g - f}{\tau} \quad (1)$$

The equilibrium state distribution function g is also called the Maxwellian equilibrium distribution function and it can be expressed as

$$g = \rho / (2\pi RT)^{3/2} \exp[-c^2 / (2RT)] \quad (2)$$

c and q are peculiar velocity and heat flux.

For the BGKX equation, Xu adopted the modern CFD kinetic flux for the left handside (LHS) terms, for the RHS Xu replaced the relaxation time τ by a strained relaxation time τ_* , [7] which allows an extended Knudsen number (Kn) range from 0 towards 0.5, thus covering the continuum to transient flow regime up to the order of BGKX-Burnett. The details of the BGKX method can be found in Ref. [3, 6-8].

Direct BGK Solver

In order to compute the flow with a high Kn number, the direct BGK solver is implemented. As shown in Eq. (1), the distribution function f is a function of three coordinates and three instantaneous velocity components and the time t : $f = f(x, y, z, t, u, v, w)$. In order to solve Eq. (1), we have to discrete the distribution function in the three coordinates and three velocity directions, then the total unknown number should be $N = N_x \cdot N_y \cdot N_z \cdot N_u \cdot N_v \cdot N_w$, which is a huge number in relation to current computer resource.

In order to reduce the computational time and computer resource, the velocity distribution function can be accurately integrated on the velocity components with weighting factors in the directions where the components of macroscopic velocity component equals zero. As a result, two new reduced distribution functions are used for the computation by replacing the original velocity distribution function.

For two-dimensional flows, the velocity distribution function equation can be accurately integrated on the velocity component with respect to w with weighting factors 1 and w^2

$$g(x, y, t, u, v) = \int_{-\infty}^{+\infty} f(x, y, z, t, u, v, w) dw \quad (3a)$$

$$h(x, y, t, u, v) = \int_{-\infty}^{+\infty} w^2 f(x, y, z, t, u, v, w) dw \quad (3b)$$

Now the reduced particle distribution functions have only five independent variables, this method dramatically decreases the unknown variables to $N = 2 \cdot N_x \cdot N_y \cdot N_u \cdot N_v$. With the reduced distribution function method, the BGK equation in a body-fitted coordinates (ξ, η) can be expressed as:

$$\frac{\partial \hat{U}}{\partial t} + \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} = S \quad (4a)$$

where

$$\hat{U} = J \begin{pmatrix} g \\ h \end{pmatrix}, F = \bar{U} \hat{U}, G = \bar{V} \hat{U}, S = \frac{J}{\tau} \begin{pmatrix} G^N - g^N \\ H^N - h^N \end{pmatrix} \quad (4b)$$

Furthermore, the unknown of the distribution function can be reduced by the discrete ordinate method, the detail of the implementation is shown in Ref. [6].

THE HYBRID BGK METHOD

Based on the BGKX method and direct BGK solver, we developed a hybrid BGKX/DBGK methodology for rarefied aerothermodynamic computations. This methodology provides an efficient solution method instead of the direct BE. Here, this method uses the domain decomposition technique to properly decompose the simulation domain into smaller sub-domains, by using an efficient local parameter, Kn_{GL} , proposed at Ref. [12]. At different regimes (near continuum or more rarefied), the hybrid method designates either the BGKX or DBGK method to be used.

Flux Coupling between BGKX and DBGK Solvers

Compared with the NS/DSMC coupling method by Schwartzentruber et al [10], the BGKX+DBGK can be coupled smoothly without flux construction because both BGKX and DBGK are solving the BGK model equation. In the BGKX solver, the velocity distribution function and the macroscopic variables are computed at the cell center by using finite volume method. In the DBGK solver, the reduced velocity distribution functions and macroscopic variables are computed at the cell vertex by using the finite difference method.

The interpolation between the two algorithm is shown in Figs. 1 and 2. In Fig. 1, the computational domain is split into two parts, the cells on the left side are the domain solved with BGKX, and the cells on the right side are those solved with DBGK. The cells with dashed lines represent the ghost cells. The circles represent the position where the BGKX variables are located and the triangles represent the positions where DBGK variable are located. Fig. 2 shows the interpolation algorithm relation between the BGKX cells and DBGK points.

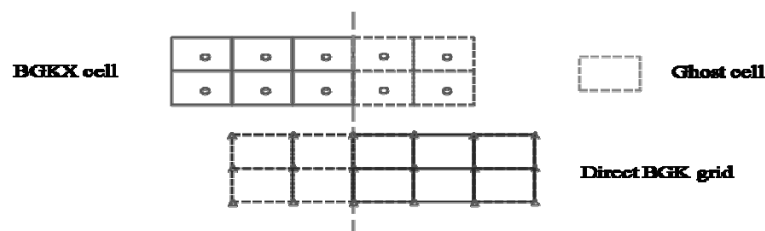


Figure 1 Interpolation diagram between cell-centered and cell-vertex variables

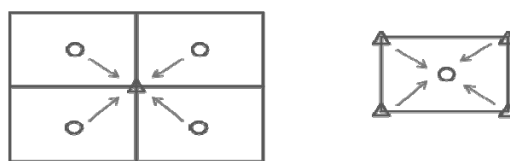


Figure 2 Interpolation between two flow solvers.

Dynamic Domain Decomposition

In order to simulate the flow efficiently, the BGKX and DBGK methods are integrated into one single hybrid code. This code automatically performs a domain decomposition to divide the whole simulation domain into several small sub-domains, and apply BGKX for continuum or near-continuum flow regimes which has a very small Knudsen number, and for regions with large Knudsen numbers DBGK should be called. A fundamental requirement for the domain decomposition criteria is it should be general and sensitive, for example, for the case of gas flows without any large rarefaction effects, the BGKX scheme shall be called throughout the flowfield to achieve high computational efficiencies; while for the case of highly rarefaction gas flows, only DBGK should be activated to yield high efficiency and high accuracy; for flows with mixed regions, the domain will automatically be divided into several sub-regions, and the boundary between regions shall be able to evolve dynamically. The last requirement is

very important for unsteady flow simulations to achieve high efficiency and accuracy. The roadmap for the coupling process is shown in Fig. 3.

Fig. 4 shows the domain decomposition for a hypersonic gas flow over a cylinder. The turquoise colored regions are for DBGK; while the blue regions need the BGKX method; the green regions are essentially buffering regions for these two methods, flux evaluations and communications are needed at these interface zones.

The continuum break-down parameter between these two regions of different rarefaction can be local Knudsen numbers defined by density, or temperature gradients; we should use the local Knudsen number [9-11] based on the local density.

$$Kn_{gl} = |\nabla\rho|L/\rho$$

The fundamentals of the domain decomposition can follow that from Ref [10], the same approach was inherited by other members from the same group, e.g. [11].

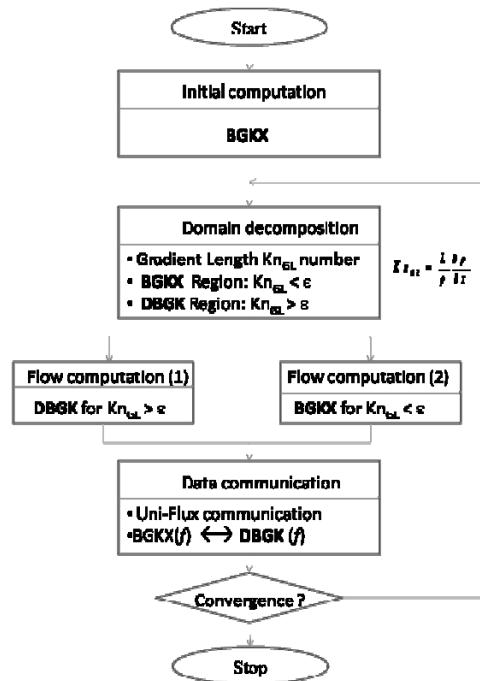


Figure 3 Roadmap of the HBGK Computation Procedure

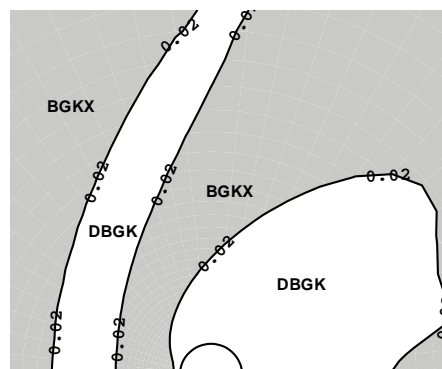


Figure 4. Domain decomposition for a hypersonic flow over a cylinder.

RESULTS FOR HBGK SOLVER

Based on the computational method described in the previous section, the HBGK code is applied to the cylinder flow. The supersonic flow around the cylinder is selected as the test case. Fig 5 shows the results for initial computation. The contour represents the density and the line shows the Kn_{GL} iso-lines. The values of the local Kn number shows that there are two regions with high Kn_{GL} . One is near the stagnation region, the other is in the shock wave region, in these regions there are larger gradient of density and pressure so we need the DBGK solver and other regions which has smaller gradients, so the BGKX is enough to predict it accurately. As shown previously in Fig. 4, the region with lighter color is the part solved with BGKX and the parts with deeper color are those for the DBGK solver.

The computational results are shown in Fig. 6 for the HBGK solver. Two case with different Kn number are computed. The case with $Kn=0.01$ is shown in Fig. 7(a), the solution from HBGK are compared with those with DBGK. The region near the shock and the wake are computed with DBGK and other parts are computed with BGKX. The computational results from HBGK agrees well with that from DBGK only. Fig. 6(b) shows the results for the same Mach number but different Kn number $Kn=0.1$. With high Kn number from the incoming flow, there exists a larger region which needs to be solved by the DBGK solver, and the rest needs the BGKX solver. The agreement between the HBGK and DBGK shows the accuracy of the current HBGK solver. As shown in Fig. 6, there are some wiggles near the buffer regions between the BGKX and DBGK solver, this might be due to the dynamic domain decomposition. In order to solve this problem, further research work are needed.

The computational efficiency is shown in Fig 7. Two different supersonic Mach number around the cylinder flow are shown in the figure. We can see the computational costs of HBGK is smaller than those with DBGK and it is larger than that for the DBGK solver, but it can keep the same accuracy as that from DBGK. For the larger Mach number, in order to keep the same computational accuracy, more points in the velocity space for the discrete ordinate method are needed for the DBGK which results in higher computational cost.

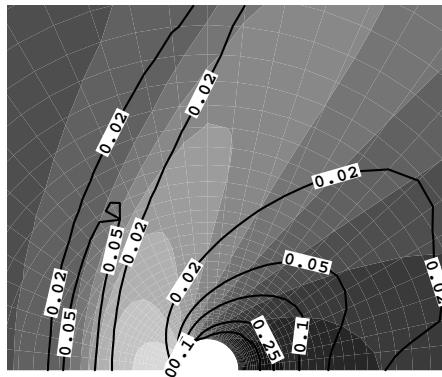


Figure 5 Density contour and the Kn_{GL} isoline ($M=1.8$ and $Kn=0.1$)

CONCLUSION

A hybrid BGK scheme was developed in this paper. The computational domain is divided into two different types of sub-domains based on the gradient-length based Kn number, and then the direct BGK solver is used to solve the sub-domains with the high Kn number and the BGKX solver is applied to the lower Kn number regions. The information between the two flow solvers is transferred through ghost cells. The hybrid scheme is applied to the rarefied flow around the cylinder at different Mach number. The computational results agree well with the full direct BGK solver and the computational efficiency has been improved.

ACKNOWLEDGEMENTS

We would like to acknowledge the support by the STTR contract (FA9550-09-C-0093) from AFOSR monitored by Dr. John Schmisser. We also want to express our thanks to the kindly help from Dr. Chunpei Cai from NMSU and Dr. Kun Xu from HKUST.

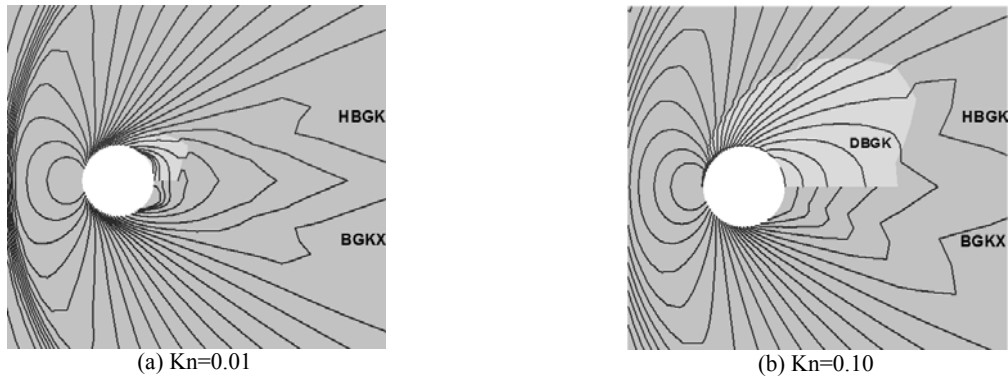


Figure 6 Pressure contour by HBGK ($M_\infty=1.8$, $Kn=0.01, 0.1$, $T_\infty=273K$, $T_w/T_\infty=2.08$)

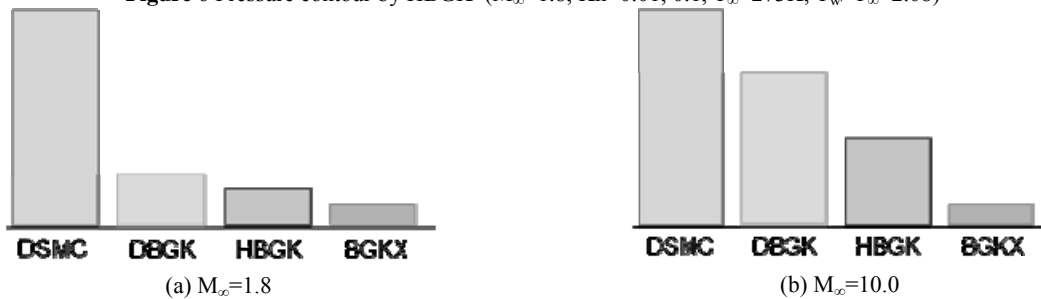


Figure 7 Computational efficiency for different solver.

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