行政院國家科學委員會專題研究計畫 成果報告

稀薄氣流與連續流一體化數值計算法研究
研究成果報告(精簡版)

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計 畫 主 持 人：黃俊誠

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中　華　民　國　96 年 10 月 30 日

行政院國家科學委員會補助專題研究計畫 ■ 成果報告 □期中進度報告

稀薄氣流與連續流一體化數值計算法研究

Unified Computational Methods for Rarefied and Continuum Flow

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中　華　民　國　96 年　10 月　30 日

稀薄氣流與連續流一體化數值計算法研究
Unified Computational Methods for Rarefied and Continuum Flow

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南華大學資訊工程系

Abstract

On Continuum flow regime, the CFD methods based on the solution of Navier-Stokes equations are used to obtain surface pressure, temperature, the flow structure around vehicle, and the coefficients of aerodynamic characteristic. For rarefied gas flow regime, which has larger Knudsen number, DSMC method has been widely used. However, for the nearly continuum flow regime, the solution of Navier-Stokes equation does not obtain accurate results and the DSMC method is difficult to deduce reliable results because the numerical results are amenable to statistical fluctuations and the computing time is expensive. It is necessary to develop an unified numerical method for simulation of rarefied, transition, and continuum flow and used for aerodynamic design of space vehicle, especially in nearly continuum flow regime. Therefore, one of the purposes of this project is to develop a numerical solver for model Boltzmann equation by integrating descrete ordinate method and CFD method for unified simulations of rarefied and continuum gas flows. After serval example testing, we conclude that the present proposed method provides an economical and efficient way to obtain accurate numerical solutions of the model Boltzmann equations for rarefied gas flows, particularly for flows with low or moderate Mach numbers. In the future works, developing an efficient hybrid method, coupling model Boltzmann and Navier-Stokes solver, and further improvement on the adaptive grid points in velocity space are warranted. The results of this project will contribute to native space project, defense technology, and industry.

Keywords: Rarefied gas dynamics, Model Boltzmann equation, Discrete ordinate method, High resolution conservative scheme, WENO scheme, Gauss-Hermite quadrature.

1. Introduction

The rarefied gas flow in transitional regime between continuum regime and free-molecule regime involved in microelectrical-mechanical devices, vacuum systems, and high altitude aerodynamics are difficult to treat either experimentally or theoretically. The physical parameter characterized the rarefied gas flow is the Knudsen number which is defined as the ratio of the mean free path to the characteristic length. The capability to accurately predict the rarefied gas flows over the complete spectrum of flow regimes is very important and desirable. The Navier-Stokes equations are inadequate to study rarefied gas flows, the kinetic theory and the Boltzmann equation needs to be used. The kinetic approach is valid in the whole range of the gas rarefaction. This is an important advantage when systems with multiscale physics are investigated.

The most commonly and well known numerical method for studying the rarefied gas flow is the direct simulation Monte Carlo (DSMC) method [1]. Applications of DSMC method to a wide variety of rarefied gas flow problems have been illustrated. However, for low Mach number or nearly continuum flow, it is difficult to deduce reliable results because the numerical results are amenable to statistical fluctuations. Instead, the difficulties in direct solving the Boltzmann equation are treating the nonlinear collision term. Recently, Kolobov and Aristov proposed the direct numerical solution (DNS) of Boltzmann equation and a unified solver for rarefied and continuum flows [2]. But, it consumes computing time and is not suitable for practical usage. Thus, instead of solving the full Boltzmann equation, one solves the kinetic model Boltzmann equation to develop a more economic and efficient way of studying rarefied gas flow.

In the present work, the discrete ordinate method was applied to the distribution function to replace its continuous dependency on the velocity space by a set of distribution functions in physical space and time but point functions in velocity space. The resulting set of differential equations can be cast into hypersonic conservation laws form with nonlinear source terms. Here, we applied the weighted essentially nonoscillatory method[3], which developed for Euler and

Navier-Stokes equations, and developed an efficient numerical method to solve model Boltzmann equation for simulation of rarefied gas flow covering the full spectrum of flow regimes.

The purpose of the three years project is to develop an efficient unified flow solver for rarefied and continuum flows, which was coupled the numerical methods for solving model Boltzmann and Navier-Stokes equations. To accelerate computation, some new methods will be developed including adaptive discrete ordinate method, scale factor quadrature, domain switching criteria, and parallel computing algorithm etc. All the new methods will be calibrated and validated with some standard test cases. The new methods developed in this project can be applied to the aerodynamic design of launch vehicle, sounding rocket, and tactical ballistic missile. Beside aerodynamic application, the new methods are useful for many technological applications, like as altitude control nozzle of satellite, vacuum pump, chemical vapor deposition in semiconductor manufacturing, and micro electro mechanical system. The results of this project will contribute to native space project, defense technology, and industry.

2. Numerical Methods

2.1 Model Boltzmann Equation

Assume there is no external force, we consider a class of model Boltzmann equations of the form

$$\frac{\partial f}{\partial t}+\vec{\mathrm{v}}\cdot\frac{\partial f}{\partial \vec{x}}=\nu\left(f^{+}-f\right),$$

where $f(\vec{x},\vec{\mathrm{v}},t)$ is the velocity distribution function which depends on space, $\vec{x}=(x,y,z)$, molecular velocity, $\vec{\mathrm{v}}=(\mathrm{v}_x,\mathrm{v}_y,\mathrm{v}_z)$ and time t. ν is collision frequency. According to the Chapman- Enskog solution to the BGK equation, the elastic collision frequency is the form

$$\nu=\frac{nkT}{\mu},$$

where T is temperature, n is number density, k is the Boltzmann constant and μ is the viscosity assumed temperature dependence

$$\mu=\mu_{ref}\left(\frac{T}{T_{ref}}\right)^{\chi}.$$

The subscript '*ref*' states the reference condition of the temperature viscosity power law. The power χ is constant for a given gas. If we assume the dependence of the viscosity on the temperature as for the Chapman- Cowling gas of inverse ς power law, we have

$$\chi=\frac{\zeta+3}{2(\zeta-1)}.$$

For Maxwell molecules, $\varsigma=5$ then $\chi=1$; thus the collision frequency is independent of temperature. The viscosity of freestream state μ_∞ relate to the freestream mean free path λ_∞ by the relation

$$\lambda_\infty=\frac{16}{5}\frac{\mu}{mn_\infty\sqrt{2\pi RT_\infty}}$$

The local Maxwellian equilibrium distribution function given by

$$f^{M}=n\left(\frac{1}{2\pi RT}\right)^{\frac{3}{2}}\exp\left(-\frac{c^2}{T}\right)$$

Since the work of Bhatnagar, Gross and Krook, the BGK model, there are serval other nonlinear model Boltzmann equations have been proposed. These include the ellipsoidal model by Holway and by Cercignani & Tironi, the polynominal and trimodal gain function models by Segal & Ferziger, and the one by Shakov and by Abe & Oguchi. The later three used rather systematic procedures to construct model equations for the nonlinear Boltzmann equation. For BGK model $f^{+}=f^{M}$, for Shakov model, we have

$$f^{+}=f^{M}\left[1+\frac{(1-\Pr)\vec{c}\cdot\vec{q}\left(c^2/RT-5\right)}{5pRT}\right]$$

Here, Pr is the Prandtl number and is equal 2/3 for a monatomic gas. The number density *n*, flow velocity $\vec{u}$, and temperature of the gas T are the first three moments of the distribution function

$$n=\int_{-\infty}^{\infty}fd\vec{\mathrm{v}}\qquad n\vec{u}=\int_{-\infty}^{\infty}\vec{\mathrm{v}}fd\vec{\mathrm{v}}$$

$$\frac{3}{2}nT=\int_{-\infty}^{\infty}\left(\vec{\mathrm{v}}-\vec{u}\right)^2 fd\vec{\mathrm{v}},$$

where R is the gas constant, $\vec{c}=\vec{\mathrm{v}}-\vec{u}$ is the peculiar velocity of the molecule.

2.2 The Discrete Ordinate Method

The distribution function is a function of 7 independent variables. In order to remove the functional dependency on the velocity space of the equations, the discrete ordinate method is applied. This method, which consists of replacing the integration over velocity space of the distribution functions by an appropriate quadrature, requires the values of the distribution function only at certain discrete velocites, that is

$$f(x,y,z,\mathrm{v}_l,\mathrm{v}_m,\mathrm{v}_n,t)=f_{l,m,m}(x,y,z,t)$$

The choice of the discrete values of velocity point is dictated by the consiferation that our final interest is not in the distribution functions themselves but in the moments. Hence, the macroscopic moments given by integrals over molecular velocity space can be evaluated by the same quadrature. The discrete ordinate method is then applied to the model Boltzmann equation for the (v_x, v_y, v_z) velocity space and the resulting differential equations are

$$\frac{\partial f_{l,m,n}}{\partial t}+\frac{\partial \mathrm{v}_l f_{l,m,n}}{\partial x}+\frac{\partial \mathrm{v}_m f_{l,m,n}}{\partial y}+\frac{\partial \mathrm{v}_n f_{l,m,n}}{\partial z}$$

$$=\nu(f^{+}_{l,m,n}-f_{l,m,n})$$

for Cartesian coordinate, and

$$\frac{\partial}{\partial t}\left(\frac{f_{l,m,n}}{J}\right)+\frac{\partial}{\partial \xi}\left(\frac{U_{l,m,n}f_{l,m,n}}{J}\right)+\frac{\partial}{\partial \eta}\left(\frac{V_{l,m,n}f_{l,m,n}}{J}\right)$$

$$+\frac{\partial}{\partial \varsigma}\left(\frac{W_{l,m,n}f_{l,m,n}}{J}\right)=\nu J(f^{+}_{l,m,n}-f_{l,m,n})$$

for general coordinate, where

$$U_{l,m,n}=\mathrm{v}_l\xi_x+\mathrm{v}_m\xi_y+\mathrm{v}_n\xi_z$$

$$V_{l,m,n}=\mathrm{v}_l\eta_x+\mathrm{v}_m\eta_y+\mathrm{v}_n\eta_z$$

$$W_{l,m,n}=\mathrm{v}_l\varsigma_x+\mathrm{v}_m\varsigma_y+\mathrm{v}_n\varsigma_z$$

Once the discrete distribution functions $f_{l,m,n}$ are solved, one can obtain all the moment integrals using Gauss-Hermite quadrature.

3. Results and Discussions

The first example we considered is the lid driven cavity flow with domain length 1. It is noted that the discretization in the phase space (physical and molecular velocity spaces) has been progressively refined to ensure accurate results. In general, in rarefied flow conditions we need a large number of discrete velocities, while the physical grid may be coarse. On the other hand, in continuum flow conditions the required number of discrete velocities may be reduced, but dense physical grids are important to achieve good accuracy. However, The present works used a non-uniform grid system with 101×101 grid points which are exponentially stretched away from the wall and the minimum grid space near the wall is depended by the Knudsen numbers. The number of discrete velocities is 26×26 for all cases. The results using Shakov model of monatomic argon gas are presented for the Mach number of moving lid is 0.9, the Knudsen numbers are 0.001, 0.0033, 0.01 and 0.1, the Reynolds number based on lid velocity and length of cavity are 1483, 148, 15, and 1.5, respectively.

Figures 1(a) to (d) show the computational results of streamline for the above cases referred the different Knudsen numbers. For the cases of *Kn*=0.001, 0.0033, 0.01 and 0.1, the streamline

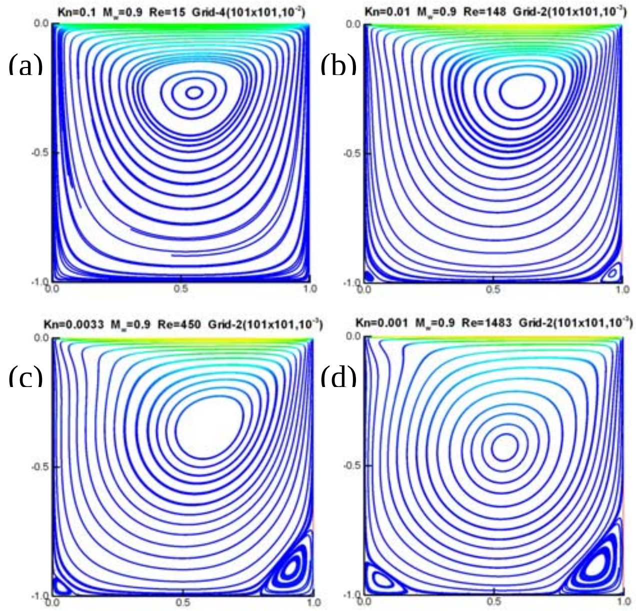

Figure 1, streamline for the cases of (a) *Kn*=0.001, (b) *Kn*=0.0033, (c) *Kn*=0.01, and (d) *Kn*=0.1

plot show a large primary vortex near the center of cavity, along with two secondary vortices at the bottom vortices at the bottom corners. The size of secondary vortex at bottom corners is decreasing by increasing the Knudsen number, and degenerated for the case of *Kn*=0.1. The effect of rarefied gas on the secondary vortex is investigated.

The second example we computed is the unsteady starting vortex flow. Early stages of

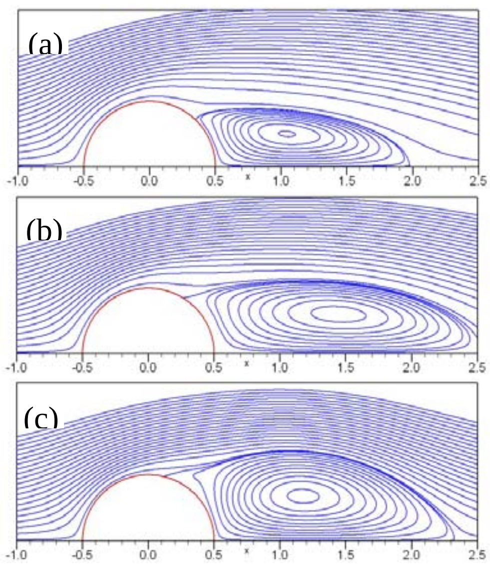

Figure 2, instantaneous streamlines for the cases of (a) *Kn*=0.01, (b) *Kn*=0.005, and (c) *Kn*=0.001.

unsteady viscous flows around an impulsively started circular cylinder at Knudsen numbers of 0.01, 0.005 and 0.001 are analysed numerically. The Mach number of upstream velocity is 0.2 for all cases. The corresponding Reynolds number, based on the upstream velocity and the diameter of the cylinder, are 33, 165 and 330, respectively. In present computations, the far field boundary is set at 20 diameters away from the center of the cylinder. A 151×181 O-type grid for the half circle domain in phyical space and 12x12 discrete points in velocity space are used.

Figure 2(a) to (c) show the results of instantaneous streamlines using BGK model with Maxwell gas at three different Knudsen number. The effect of Knudsen number on the wake behind a circular cylinder was presented. It depicts the length and width of recirculating zones varying with Kundsen number changed.

The third example is the development of dilute flow over a vertical plate that is inserted into a uniform flow at zero time. The length of the plate is 1, located at x =0, the computational

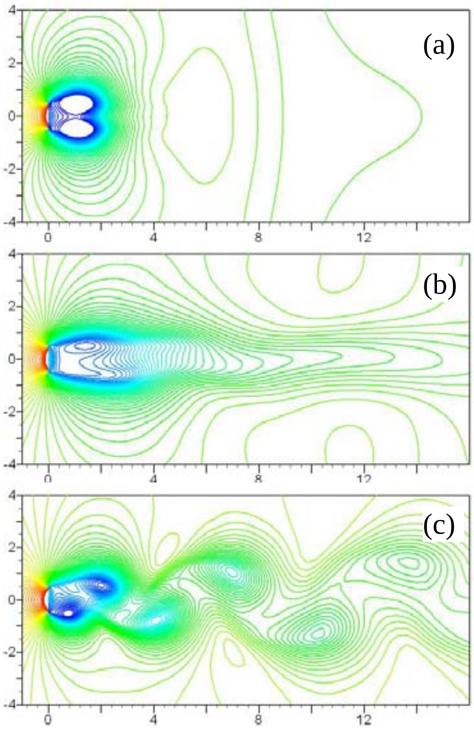

Figure 3, flow direction lines for nondimensional time (a) t =14, (b) t =66, and (c) t =146.

domain covered from –10 to 40 in x direction and from –10 to 10 in y direction. A two blocks grid system with 51x121 and 201x121 points is used. The case is for the flow of monatomic Maxwell gas with BGK model at Mach number 0.9, Knudsen number 0.005, and corresponding Reynolds number 66. The surface of the plate is diffusely reflecting with full accommodation to a temperature equal to the freestream temperature.

Figure 3(a) to (c) illustrated the results of instantaneous flow direction lines at time 14, 66, and 146. When the plat is inserting into the flow, a disturbing wave move upstream and downstream, and wave diffracting around the edges. The vortices formed behind the plate after a short period. The flow remains symmetrical at time 66. Some asymmetry develops near the downstream stagnation point. The asymmetry grows and the flow deflection occurred near the center of wake, and then fully developed wake is attained. Figure 4 shows the local Knudsen number of the flow at fully developed wake instability.

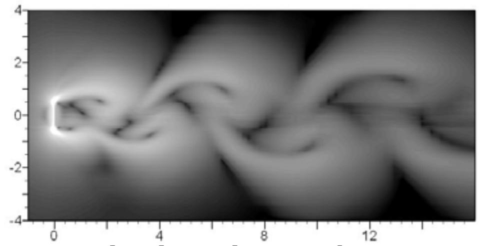

Figure 4, local Knudsen number at time 146.

4. Concluding Remarks

Based on the above computed examples, we conclude that the present proposed method provides an efficient way to obtain numerical solutions of the model Boltzmann equations for rarefied gas flows, particularly for flows with low or moderate Mach numbers. The present method although capable of treating high Mach number flows, but is very computationally expensive. In the future works, we will develop an efficient hybrid method, coupling model Boltzmann and Navier-Stokes solver to an unified gas flow solver, to treat high Mach number flows. Also, further improvement on the adaptive grid points in velocity space is warranted.

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可供推廣之研發成果資料表

□ 可申請專利　■ 可技術移轉　日期：96 年 10 月 30 日

國科會補助計畫	計畫名稱：稀薄氣流與連續流一體化數值計算法研究 計畫主持人：黃俊誠 計畫編號：NSC 95－2221－E－343 －005－　學門領域：航太
技術/創作名稱	稀薄氣體流模擬軟體
發明人/創作人	黃俊誠
技術說明	中文： 稀薄氣體流模擬軟體應用分立座標法、Scaling Factor Gauss-Hermite 積分法、三階與四階準確度 WENO 算則解 Boltzmann 模型方程式（包含 BGK、Shakov 與 Ellipsoidal 三種模型）。
	英文： The rarefied gas simulation code solves the model Boltzmann equations, including BGK, Shakov, and Ellipsoial model), with discrete ordinate method, Scaling Factor Gauss- Hermite quadrature, and high order accurate WENO schemes.
可利用之產業及可開發之產品	本計畫成果除了應用於飛行器氣動力學研究外，也可以推廣應用於衛星姿態控制噴嘴、真空泵浦、化學氣相沉積、以及微機電系統等科學及工業上。在太空計畫、國防科技與產業發展等均能有所助益。
技術特點	本項技術 CFD 方法解 Boltzmann 模型方程式(包含 BGK、Shakov 與 Ellipsoidal 三種模型)，應用於稀薄氣體流模擬與分析。尤其應用在近連續體流區域流，以及中、低馬赫速流場模擬時，更能顯現其計算效率與準確度。
推廣及運用的價值	本軟體計算效率高，並可處理複雜的幾何外形，可應用於近連續體流至稀薄流場模擬。

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