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Assessment of the cubic Fokker–Planck–DSMC hybrid method for hypersonic rarefied flows past a cylinder

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ABSTRACT

Hypersonic vehicles experience a wide range of Knudsen number regimes due to changes in atmospheric density. The Direct Simulation Monte Carlo (DSMC) method is physically accurate for all flow regimes, however it is relatively computationally expensive in high density, and low Knudsen number regions. Recent advances in the Fokker–Planck (FP) kinetic models have addressed this issue by approximating the particle collisions involved in the Boltzmann collision integral with continuous stochastic processes. Furthermore, a coupled FP–DSMC solution method has been devised aiming at a universally efficient yet accurate solution algorithm for rarefied gas flows. Well known Lofthouse case of a generic hypersonic flow about a cylinder (Mach 10, Kn 0.01, Argon) is selected to investigate the performance of a hybrid FP–DSMC implementation. The effect of molecular potential on the accuracy of the scheme is mainly analyzed. Furthermore, spatial resolution of cubic FP scheme is studied. Finally, detailed study of accuracy and efficiency of FP–DSMC hybrid scheme is discussed. It is found that the presented adaptive grid together with the FP–DSMC method results in a factor of six speed up for considered hypersonic flow about a cylinder.

1. Introduction

Rarefied gas dynamics is concerned with flows at low density where the molecular mean free path is not negligible. Under these conditions, the continuum assumption breaks down and the gas no longer behaves according to the conventional hydrodynamics. Important modifications in the aerodynamic and heat transfer characteristics occur which are associated with the basic molecular structure of the gas. The degree of rarefaction is generally characterized through the Knudsen number $\mathrm{Kn} = \lambda/\mathrm{L}$, where λ is the mean free path of the gas and L is a characteristic length scale. The flow regime is classified as free molecular, transitional, and continuum, depending on the Knudsen number [1]. It is generally accepted that free molecular flow is an accurate assumption for $\mathrm{Kn} \geq 10$, whereas $\mathrm{Kn} \ll 1$ chracterizes the hydrodynamic limit. In the latter case, one can disregard microscopic phenomena in the gas and consider only macroscopic fields such as density, velocity and temperature as the relevant physical quantities. Due to the sufficiently large number of collisions the distribution $\mathcal{F}(\mathbf{V})$ of particle velocity remains close to an equilibrium distribution, and the conventional Navier–Stokes or Euler equations are appropriate models. Yet as the Knudsen number increases, the local velocity distribution may depart significantly from equilibrium, and the flow may not be accurately described by the Navier–Stokes equations. Therefore, the Boltzmann equation should be regarded as the governing model [1]. The Boltzmann equation provides the evolution of the velocity distribution according to

$$\frac{\mathrm{D}\mathcal{F}}{\mathrm{D}t} = \frac{1}{m}\int_{R^3}\int_0^{4\pi}\left(\mathcal{F}(\mathbf{V}^*)\mathcal{F}(\mathbf{V}_1^*) - \mathcal{F}(\mathbf{V})\mathcal{F}(\mathbf{V}_1)\right)g\sigma(\theta, g)\mathrm{d}\theta\mathrm{d}^3\mathbf{V_1} \tag{1}$$

with $\mathrm{D}(\ldots)/\mathrm{D}t = \partial(\ldots)/\partial t + V_i\partial(\ldots)/\partial x_i + G_i\partial(\ldots)/\partial V_i$. Here the m is the mass of a single gas molecule, the velocity pair $(\mathbf{V}_1^*, \mathbf{V}^*)$ is the post collision state of the pair $(\mathbf{V}_1, \mathbf{V})$, σ is the differential cross section of the collision, θ the solid angle which provides the orientation of the post collision relative velocity vector and $g = |\mathbf{V} - \mathbf{V}_1|$. Furthermore, $\mathbf{G}$ represents the external force normalized by the molecular mass. For engineering applications, the direct numerical solution of the Boltzmann equation may become computationally demanding, due to non-linearity of the collision operator and the high dimensionality of the solution domain.

Alternative to the direct discretization of the distribution function, particle Monte-Carlo approximations can deal with high dimensionality very effectively. In particular, solution algorithms based on DSMC, employ computational particles and Monte-Carlo

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techniques to simulate the gas flow according to the Boltzmann equation. As a stochastic particle method, DSMC is the most mature and commonly used high fidelity simulation method for rarefied gas flows [1]. The DSMC method has evolved over 50 years into a powerful numerical technique for the computation of thermochemical non-equilibrium gas flows [2–4]. There exists a number of implementations of DSMC method, including DS2V/3V (G.A. Bird, Australia), MONACO (University of Michigan, USA), SMILE (Khristianovich Institute of Theoretical, Russia), DAC (NASA Langley Center, USA), MGDS (University of Minnesota, USA), HAP (Airforce, USA), openFoam (dsmcFOAM), SPARTA (Sandia national laboratories, USA) [5–11]. More recently, SPARTA[1] was developed at Sandia National Laboratories as a general-purpose 3D DSMC simulator designed to run efficiently on parallel computers. It is an open-source code, distributed freely under the terms of the GNU Public License and was released in 2014 [11].

While physically accurate for ideal gas flows over the entire range of rarefaction, standard DSMC becomes expensive as the flow approaches the hydrodynamic limit. Therefore, DSMC may not be an appropriate tool due to the computational expense for flows with a wide range of local Knudsen number, such as hypersonic entry flows. This gives a very good motivation for hybrid methods, in which different models are employed for different Knudsen regimes. Traditional hybrid methods rely on coupling continuum model, mainly the Navier–Stokes equations, with the high fidelity non-equilibrium solvers [12,13]. Continuum Computational Fluid Dynamics (CFD) method is assigned to the near equilibrium regions while DSMC is only applied to high Knudsen sub-domains. However, the CFD-DSMC scheme deals the two-way coupled information transfer between CFD and DSMC domains. It is complex and requires significant algorithm developments. In particular, feeding the noisy Monte-Carlo type information from the DSMC solution to the boundary of the continuum solver is troublesome.

Another type of hybrid approach is given by coupling DSMC with near-equilibrium particle methods [14–16]. These approaches rely on DSMC type particle updates at high Knudsen number regimes whereas continuum particle updates are enforced elsewhere. These methods can handle very strong coupling between the two flow regimes. They allow simpler code development, as there is no need to integrate two different simulation schemes in the same code. However, these techniques are prone to significant errors associated with numerical diffusion, including effects of artificial viscosity, thermal conductivity and mass diffusion resulting from free-molecular fluxes between adjacent cells [17].

Recently, an alternative stochastic particle scheme was proposed by Jenny et al. and Gorji et al., where the collision process underlying the Boltzmann equation is approximated by a Fokker–Planck (FP) kinetic model [18–20]. In the cubic FP approach, the Boltzmann equation is reduced to a drift and diffusion stochastic process, where the particles follow independent stochastic paths. That leads to a high computational efficiency at low Knudsen numbers where the flow is dominated by intermolecular collisions. The drift and diffusion coefficients in the cubic FP model are then computed based on consistency relations with respect to the Boltzmann collision integral. Furthermore, the hybrid FP–DSMC approach was subsequently developed providing an easy to develop, accurate yet efficient simulation tool [21–23]. However, the performance and efficiency of the FP–DSMC approach has to be further analyzed especially with regard to application of molecular potentials. This is in particular important since it has been shown that the cubic FP model does not provide accurate shock profiles unless Maxwell type molecules are assumed [24].

[1] Stochastic Parallel Rarefied-gas Time-accurate Analyzer.

This paper aims for a detailed study of FP–DSMC simulations with focus on the effect of molecular potentials on the accuracy and efficiency of the model. First, the standard DSMC and cubic FP results are compared with each other in order to investigate the influence of molecular potential on hypersonic flow phenomena. Second, the requirement for the FP spatial resolution is discussed based on the maximum gradient of macroscopic values. The FP solutions with three different grid configurations are compared. Finally, the FP–DSMC hybrid simulation are performed with Maxwell and VHS molecular models, using two different grid configurations.

2. Numerical methods

2.1. DSMC

The main idea behind DSMC is to employ computational particles as Monte-Carlo realizations of the distribution. These particles, which can be regarded as representatives of a huge number of real molecules, evolve in a two step algorithm consistent with the Boltzmann equation. More precisely, the main principle of the DSMC is the splitting of the evolution into two sequential stages: free molecular translation and intermolecular collisions. The collision pairs are picked from the same computational cell. Therefore, the cell sizes should resolve the local mean free path of the gas. Accordingly, the splitting requires that the time step size honours the mean collisions time. The DSMC algorithm consists of translational movement of particles, application of boundary conditions, calculation of collisions, and sampling particle quantities for macroscopic flow variables [1,4]. Details are summarized in the flowchart 2. The DSMC simulations conducted in the present article are performed with SPARTA.

2.2. Cubic Fokker–Planck model

The efficiency of the FP based particle simulations can be achieved due to the fact that the resulting model equations are continuous stochastic differential equations in the velocity space. In the following we review the basic elements of the cubic FP model (for more details see e.g. [19]). The FP kinetic model is an approximation of the Boltzmann collision operator

$$\left(\frac{\partial \mathcal{F}}{\partial t}\right)_{coll} \approx -\frac{\partial}{\partial V_i}\left(A_i \mathcal{F}\right) + \frac{1}{2}\frac{\partial^2}{\partial V_j \partial V_j}\left(D^2 \mathcal{F}\right) \tag{2}$$

by a drift-diffusion process in the phase space. Here, $\mathbf{A}$ and D represent the drift and diffusion coefficients which in general may be functions of $\mathcal{F}$ and $\mathbf{V}$. In the cubic FP model, the drift coefficient is derived from a polynomial ansatz

$$A_i = c_{ij} v'_j + \gamma_i \left(v'_j v'_j - \frac{3kT}{m} \right) + \Lambda \left(v'_i v'_k v'_k - \frac{2q_i}{\rho} \right) \tag{3}$$

as a function of the fluctuating velocity v'. The coefficients $\mathbf{c}$ and γ are derived such that exact relaxation of the viscous stresses σ and heat fluxes $\mathbf{q}$ are obtained for Maxwell molecules. The cubic coefficient Λ ensures stability of the equation as v' approaches infinity. The diffusion coefficient, D is found to be:

$$D = \sqrt{\frac{2kT}{m\tau}} \tag{4}$$

based on the Langevin equation [18]. Time scale $\tau = 2\mu/p$ is employed in the cubic FP model which is proportional to the mean collision time of Maxwell molecules. Since the relaxation time scale τ depends only on the equilibrium quantities, certain limitations for realistic molecular potentials will be expected.

Eqs. (3) and (4) already close the cubic FP approximation. But in order to develope a particle based numerical scheme, the kinetic