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A methodology for hybrid simulation of Rarefield and continuum flow regimes

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ABSTRACT

A hybrid procedure consisting of a high order continuum (HOC) model and the direct simulation Monte-Carlo (DSMC) solver is proposed in this paper, as it represents a promising approach for seamless computation of hypersonic flows in all regimes. This approach also allows the effects of thermophysics (thermal and chemical non-equilibrium) and turbulence to be included so that gas interactions can be modeled much more easily than in other approaches. Such hybrid procedures can also be developed into robust and efficient parallel computing tools for practical 3D computations. The main idea behind the proposed HOC/DSMC methodology consists of incorporating the physically realizable and computationally stable version of the Burnett equations into hypersonic codes that have the capability for calculating non-equilibrium chemistry and temperature. We explore the feasibility of simplified, yet accurate and numerically stable, versions of the Burnett equations. We discuss such a model in detail, providing an analysis of its stability and performance for Alsmeyer's shock wave problem and hypersonic flow over a sphere. We also report on the performance of the DSMC component of the proposed hybrid scheme.

1. Introduction

Hypersonic flows over space vehicles produce flow fields with local Knudsen numbers, Kn, which may lie in all the three regimes – continuum, transition, and rarefied. The Navier–Stokes (NS) equations and the direct simulation Monte-Carlo (DSMC) methods can accurately and efficiently model the flows in the continuum and rarefied regimes, respectively. Of these two approaches, i.e., continuum and kinetic, the latter considers an ensemble of small particles or molecules whose distribution function can be determined as a solution of the Boltzmann equation. The former approach is based on the representation of the gas as a fluid continuum governed by the mass, momentum, and energy conservation laws. Although, theoretically, the kinetic approach is appropriate for simulating gas flows in any regime; in practice, it can require prohibitively large computational resources if the gas flow is dense. DSMC remains an efficient numerical technique for solving the Boltzmann equation [1]. It enables the computation of flows with Knudsen numbers $Kn \geq 0.001$ for 2D problems and $Kn \geq 0.01$ in the 3D case, i.e., almost nearly down to the continuum regime [2,3]. (Of course, these Kn values, 0.001 and 0.01, are approximate.) Here, $Kn = \lambda/L$, where λ is the mean free path of the molecules and L is the characteristic length scale of the flow. Nevertheless, DSMC computations are still too expensive in many cases, especially for 3D engineering applications. Also, being a rather efficient tool for supersonic and particularly hypersonic flows [3], they become more resource-consuming for low Mach number subsonic flows, due to difficulties with boundary condition implementation on subsonic inflow/outflow boundaries [4]. Furthermore, obtaining gas interactions with DSMC is a difficult task. The continuum approach is much cheaper and more versatile in these regards. There is, therefore, a strong motivation for its utilization at the low Kn values.

The traditional continuum model is based on the Navier–Stokes equations, which are the first order approximation to the Boltzmann equation with respect to Kn as the small parameter in the asymptotic expansion. Coupled with no velocity slip/no temperature jump solid wall boundary conditions, they are valid if the Knudsen number is smaller than 0.001. More rarefied flows should be described using the Navier–Stokes equations with velocity slip/temperature jump boundary conditions. However, the flows in the transitional regime ($0.1 < Kn < 10$) require higher order

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Nomenclature

Y_s	Mass concentration of species s
D_s	Effective diffusion coefficient for species s..... m^2/s
D_{sk}	Multicomponent diffusion coefficient
e	Elementary electronic charge, 1.6022×10^{-19} C or total energy per unit mass
E	Electronic field, function (space, time)..... V/m
E_e	Electronic translational energy per unit volume
ϵ_o	Permittivity of free space, 8.8542×10^{-12} F/m
h^o	Enthalpy of formation
k	Boltzmann constant, 1.3807×10^{-23} J/K
L	Characteristic length
M_e	Electron mass, 9.1094×10^{-31} kg
M	Mach number, Molecular weight
N	Number density
p	Pressure
q	Charge, C, or heat flux vector
Q_{rad}	Radiation heat loss term
Q	Energy exchange between modes
T	Translational temperature
T_v	Vibrational temperature
u^j	Mass-averaged velocity component in 3 dimensions m/s, $j = 1$ to 3
u_s	Average or mean velocity
V	Random or peculiar velocity or diffusion velocity
Z_s	Ionic valency, -1 for electrons, 1 for single-ionized positive ions
τ	Relaxation time
τ^{ij}	Viscous shear stress
x^j	Position vector in 3 dimensions, $j = 1$ to 3
X	Mole fraction
ν	Collision frequency
ν^*_{er}	Effective collision frequency of electrons with diatomic molecules (heavy particles)
Θ_d	Characteristic temperature of dissociation
Θ_v	Characteristic temperature of vibration
Γ	Flux density
ω_{pe}	Electron plasma frequency, 5.64×10^4 rad/s
ω	Source or sink of species
η'	Thermal conductivity coefficient
σ	Collision cross-section
ρ_n	State density in the nth vibrational level
ρ	Total density..... kg/m^3

Subscripts

D	Debye
e	Electron
I	Ion
n, m	Species indices in quantum level
R	Diatomic molecule (heavy particle)
s	Species
v	Vibration
∞	Freestream conditions

Superscripts

i, j	ith and jth components in general orthogonal coordinates

models, the most well-known being the Burnett equations obtained as second order approximations with respect to Kn. Though there are some difficulties with the stability of their solutions and the development of relevant solid wall boundary conditions, recent enhancements [5] allow the consideration of the (modified) Burnett equations as a potential continuum model for transitional flows. In recent years, Burnett equations have been successfully employed to compute 3D hypersonic flows in continuum-transition regimes [6], although it has been difficult to compute flows for $Kn > 1$ with the approach.

The other HOC equations, such as Eu's [7] and Grad's 13-moment equations [8], are significantly more expensive to compute than the Burnett equations, and have been tested only for 1D and for 2D geometrically simple problems. Another approach is due to Aristov and Tcheremissin [9], wherein a special quadrature formula is employed for the collision integral on the right-hand side. This method has been applied to solve 2D problems involving a mono-atomic gas. Application of the approach to gases with internal degrees of freedom is problematic at the moment, given the difficulty with the inclusion of chemical reactions.

A detailed description of the DSMC method and the direct Boltzmann solver of Aristov and Tcheremissin, as well as the discussions of their relative advantages and disadvantages, can be found in the references. However, none of the approaches can efficiently compute all the flow regimes that may be present on a space vehicle in hypersonic flight.

A careful examination of the options has led us to the conclusion that a hybrid high order continuum/direct simulation Monte-Carlo (HOC/DSMC) solver represents the most promising approach for seamless computation of hypersonic flows in all regimes. Moreover, the procedure can easily be extended to include the effects of thermophysics (thermal and chemical non-equilibrium) and turbulence. In addition, the proposed hybrid codes can be developed to be robust, stable, and efficient on parallel computing platforms for practical 3D computations. The main idea behind the proposed HOC/DSMC methodology is described below.

The hybrid method requires for each cell: (a) the determination of which approach – continuum or particle – is valid, and: (b) the development of interface boundary conditions, which basically connect the two approaches at the cell interface. For each cell, whether the continuum model breaks down or not is determined by employing a switching (or breakdown) parameter. There are a few switching criteria that have been proposed in the literature [10,11], each of which is based on the premise that the Navier–Stokes equations are not valid when the nonlinear terms in the Chapman–Enskog expansion become important – when the velocity distribution function deviates from its equilibrium state by some degree. One can use the criteria based either on the local Knudsen number or on the ratio of the maximum shear stress to the maximum heat-flux. However, the effectiveness of various possible criteria needs to be evaluated by numerical experiments. Limited amount of work has been carried out on this issue, but see Boyd [12] for a short review of breakdown prediction. In the present study, the gradient-length-local Knudsen number discussed by Boyd has been used, although other options, such as the parameter involving direct evaluation of heat flux tensor elements, have also been tested.

Once the cells in which the continuum model holds have been identified using the switching criteria, the calculations for the rest of the cells in the flow field are performed with the DSMC method. The next important issue in the hybrid method is connecting the continuum cells with the particle cells on the interface in a seamless fashion. On one hand, the numerical fluxes calculated by the continuum approach must be transformed into particle fluxes for the DSMC method. On the other, the field values of macroscopic quantities such as density, velocity, pressure, and

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