Journal of Computational Physics 232 (2013) 468–481

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

A non-equilibrium surface reservoir approach for hybrid DSMC/Navier–Stokes particle generation

K.A. Stephani *, D.B. Goldstein, P.L. Varghese

Department of Aerospace Engineering, The University of Texas at Austin, USA

ARTICLE INFO

Article history:
Received 18 November 2011
Received in revised form 16 August 2012
Accepted 20 August 2012
Available online 1 September 2012

Keywords:
Hybrid methods
Generalized Chapman–Enskog Theory
Particle generation
Non-equilibrium flows

ABSTRACT

An approach for the generation of particles at a hybrid Navier–Stokes/DSMC interface is presented for simple gases and gas mixtures with internal degrees of freedom. DSMC particles generated at a hybrid boundary are assigned thermal velocities using a non-equilibrium surface reservoir approach, in which the fluxes of mass, momentum and energy determined from the Navier–Stokes solution are used to prescribe the appropriate velocity distribution function used in the DSMC particle generation. The non-equilibrium surface reservoir approach is first outlined for a simple (single-species, monatomic) gas, and is then extended to gas mixtures with internal degrees of freedom, in which additional diffusion and internal heat flux terms are included in the Generalized Chapman–Enskog formulation of the perturbation. The significance of the diffusion, shear stress and heat flux breakdown parameters used to compute the perturbation are examined at a hybrid interface within non-equilibrium boundary layer flow, as well as within the breakdown region near a normal shock, in a five-species air gas mixture. The validity of the Chapman–Enskog perturbation at each of these hybrid interfaces is assessed by comparison with the Generalized Chapman–Enskog perturbations. Although a hybrid flowfield solution is not presented, this work provides a rigorous approach for non-equilibrium particle generation involving general hybrid particle/continuum studies of hypersonic flows.

1. Introduction

The quality of a hybrid solution involving direct simulation Monte Carlo (DSMC) and Navier–Stokes solvers relies on the accurate representation of the flowfield across the hybrid interface. In previous hybrid particle/continuum studies, the transfer of information from the Navier–Stokes solution to the DSMC solver is made almost exclusively through the velocity distribution function, which is used to prescribe the thermal velocities of particles generated at the hybrid interface. When the flowfield at the location of the hybrid interface is in equilibrium, the particle thermal velocities may be prescribed from a Maxwellian distribution. In contrast, DSMC particles that are generated at an interface within a non-equilibrium region follow a perturbed velocity distribution which, for small departures from equilibrium, may be described by the Chapman–Enskog distribution function.

Deschenes et al. [1,2] have recently devised a hybrid approach to include the additional effects of thermal (translational–rotational) non-equilibrium in determining the breakdown location in hypersonic flows with internal energy. This is accomplished through the use of a gradient-based Knudsen number [3] as well as a breakdown parameter based on translational–rotational non-equilibrium. These studies also suggest the generation of particle rotational energies from

* Corresponding author. Address: Department of Aerospace Engineering, The University of Texas at Austin, 210 E. 24th Street, 1 University Station, C0600 Austin, TX 78712, USA. Tel.: +1 512 471 7593; fax: +1 512 471 3788.

E-mail address: kelly.stephani@mail.utexas.edu (K.A. Stephani).

0021-9991/$ - see front matter
http://dx.doi.org/10.1016/j.jcp.2012.08.017

the rotational (Boltzmann) energy distribution obtained from the continuum solution, but the particle thermal velocities are sampled from the regular Chapman–Enskog distribution as outlined in Garcia and Alder [4], valid for only simple (single-species, monatomic) gases. This work aims to incorporate the effects of thermal non-equilibrium (translational–rotational and translational–vibrational) on the hybrid particle sampling process in a rigorous way through use of the Generalized Chapman–Enskog distribution. This extension allows for the sampling of both thermal velocities as well as internal energies from the perturbed (i.e., *near*-equilibrium) Maxwell–Boltzmann distribution, and a new set of breakdown parameters are obtained through this rigorous formulation.

Particles generated at the hybrid interface may be introduced into the computational domain using either a volume reservoir or surface reservoir approach [5,6]. The volume reservoir approach populates reservoir or 'ghost' cells with randomly distributed simulation particles whose thermal velocities are prescribed according to the appropriate velocity distribution function. These particles are allowed to move within the reservoir cells and into the computational domain during the initial particle creation. Particles that enter the computational domain are used in the simulation, while any particles remaining in the reservoir cells are deleted.

The surface reservoir is an alternative approach to hybrid particle generation. A surface reservoir may be thought of as a surface which emits randomly distributed particles at a rate that is consistent with the macroscopic properties of the fluid. The surface reservoir approach may be more computationally efficient than the volume reservoir approach, since all particles generated at the hybrid domain boundary are used in the simulation. The velocity distribution function describing the thermal velocities of these particles is formulated by computing the distribution of particles in an infinite reservoir which would cross the surface reservoir boundary and enter into the computational domain during a single timestep. The tangential thermal velocity components of particles emitted from a surface reservoir located in an equilibrium flowfield region follow a Maxwellian distribution, as in the case of the volume reservoir. However, the thermal velocity component normal to the surface reservoir follows a *one-sided* Maxwellian distribution.

The current work seeks to extend the surface reservoir approach to particles generated in a non-equilibrium flowfield region. The non-equilibrium surface reservoir distribution function is derived first for a simple gas assumed to follow a Chapman–Enskog distribution (Section 2.1), and a general approach for particle sampling from this distribution is outlined at the end of this section and Appendix A. This surface reservoir approach is then extended to a gas mixture with internal degrees of freedom by way of the Generalized Chapman–Enskog framework (Section 2.2 and Appendix B), and a general approach for particle sampling from these distributions is provided at the end of Section 2.2. In Section 3 a simple analysis is presented in which the significance of the diffusion flux, shear stress and heat flux contributions to the Generalized Chapman–Enskog perturbation are assessed for a hybrid interface within a non-equilibrium boundary layer flowfield (Section 3.1), as well as within the breakdown region near a normal shock (Section 3.2). A summary of this work and conclusions are provided in Section 4.

2. Particle generation using a non-equilibrium surface reservoir approach

2.1. Surface reservoir approach for a simple gas

The surface reservoir approach may be thought of as a surface which emits randomly distributed particles at a rate that is consistent with the macroscopic properties of the fluid right at the surface. In equilibrium conditions (i.e., $\tau_{ij} = q_i = 0$), the thermal velocity components tangential to the fluxing surface may be generated from a Maxwellian distribution, however the thermal velocity component normal to the fluxing surface is prescribed from a *one-sided* Maxwellian distribution [6,7]. Under non-equilibrium conditions (i.e., $\tau_{ij}, q_i \neq 0$), the Chapman–Enskog distribution should be employed for cases in which the flow exhibits a small departure from equilibrium [4,5,8]. Garcia and Alder presented an acceptance–rejection algorithm for generating particle velocities from a Chapman–Enskog distribution within a volume reservoir [4]. To generate particles under non-equilibrium conditions using a surface reservoir approach, we must first derive the appropriate velocity distribution for a non-equilibrium surface reservoir.

Consider a simple gas inside a reservoir extending from $(-\infty < x \leqslant 0)$ which follows a Chapman–Enskog distribution. The velocity distribution describing the particle thermal velocities within the reservoir may be expressed as [9–11]:

$$f^{(1)}(\mathbf{C}) = f^{(0)}(\mathbf{C})\Gamma(\mathbf{C}), \tag{1}$$

where $f^{(0)}(\mathbf{C})$ is the equilibrium Maxwellian distribution defined by:

$$f^{(0)}(\mathbf{C}) = \left(\frac{\beta}{\pi^{1/2}}\right)^3 \exp\left[-(\beta^2 C_x^2 + \beta^2 C_y^2 + \beta^2 C_z^2)\right]. \tag{2}$$

The quantity $\Gamma(\mathbf{C}) = 1 + \phi_{CE}(\mathbf{C})$ is the perturbation function describing the small departure from the equilibrium state which may be expressed as:

$$\Gamma(\mathbf{C}) = 1 + (q_x\mathcal{C}_x + q_y\mathcal{C}_y + q_z\mathcal{C}_z)\left(\frac{2}{5}\mathcal{C}^2 - 1\right) - 2(\tau_{xy}\mathcal{C}_x\mathcal{C}_y + \tau_{xz}\mathcal{C}_x\mathcal{C}_z + \tau_{yz}\mathcal{C}_y\mathcal{C}_z) - \left(\tau_{xx}\mathcal{C}_x^2 + \tau_{yy}\mathcal{C}_y^2 + \tau_{zz}\mathcal{C}_z^2\right), \tag{3}$$

where, for compactness, the product of the thermal velocity components and the inverse most probable thermal speed is expressed as $\mathcal{C}_i = C_i\beta$. The variable $\mathcal{C}_i$ is the scaled thermal velocity component in the direction i where