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Continuum Formulation for Non-Equilibrium Shock Structure Calculation

Kun Xu[1,*] and Eswar Josyula[2]

[1] *Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*
[2] *Air Force Research Laboratory, 2210 Eighth Street, Wright-Patterson AFB, OH 45433, USA.*

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Abstract. Are extensions to continuum formulations for solving fluid dynamic problems in the transition-to-rarefied regimes viable alternatives to particle methods? It is well known that for increasingly rarefied flow fields, the predictions from continuum formulation, such as the Navier-Stokes equations lose accuracy. These inaccuracies are attributed primarily to the linear approximations of the stress and heat flux terms in the Navier-Stokes equations. The inclusion of higher-order terms, such as Burnett or high-order moment equations, could improve the predictive capabilities of such continuum formulations, but there has been limited success in the shock structure calculations, especially for the high Mach number case. Here, after reformulating the viscosity and heat conduction coefficients appropriate for the rarefied flow regime, we will show that the Navier-Stokes-type continuum formulation may still be properly used. The equations with generalization of the dissipative coefficients based on the closed solution of the Bhatnagar-Gross-Krook (BGK) model of the Boltzmann equation, are solved using the gas-kinetic numerical scheme. This paper concentrates on the non-equilibrium shock structure calculations for both monatomic and diatomic gases. The Landau-Teller-Jeans relaxation model for the rotational energy is used to evaluate the quantitative difference between the translational and rotational temperatures inside the shock layer. Variations of shear stress, heat flux, temperatures, and densities in the internal structure of the shock waves are compared with, (a) existing theoretical solutions of the Boltzmann solution, (b) existing numerical predictions of the direct simulation Monte Carlo (DSMC) method, and (c) available experimental measurements. The present continuum formulation for calculating the shock structures for monatomic and diatomic gases in the Mach number range of 1.2 to 12.9 is found to be satisfactory.

Key words: Non-equilibrium flow; bulk viscosity; kinetic scheme; shock structure.

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[*] Correspondence to: Kun Xu, Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong. Email: `makxu@ust.hk`

1 Introduction

The classification of the various flow regimes based on the dimensionless parameter, the Knudsen number, is a measure of the degree of rarefaction of the medium. The Knudsen number Kn is defined as the ratio of the mean free path to a characteristic length scale of the system. In the continuum flow regime where $\mathsf{Kn} < 0.001$, the Navier-Stokes equations with linear relations between stress and strain and the Fourier's law for heat conduction are adequate to model the fluid behavior. For flows in the continuum-transition regime $(0.1 < \mathsf{Kn} < 1)$, the Navier-Stokes equations are known to be inadequate. This regime is important for many practical engineering problems, such as the simulation of microscale flows [12] and hypersonic flow around space vehicles in low earth orbit [15]. Hence, there is a strong desire and requirement for accurate models which give reliable solutions with lower computational costs. The Boltzmann equation describes the flow in all flow regimes; continuum, continuum-transition and free molecular.

The numerical techniques available for solving the Boltzmann equation can be classified into particle methods and continuum methods. The direct simulation Monte Carlo (DSMC) [7] falls in the category of particle methods. The DSMC method is a widely used technique in the numerical prediction of low density flows. However, in the continuum-transition regime, where the density is not low enough, the DSMC requires a large number of particles for accurate simulation, which makes the technique expensive both in terms of the computation time and memory requirement. At present, the accurate modeling of realistic configurations, such as aerospace vehicles in three dimensions by the DSMC method for $\mathsf{Kn} << 1$, is beyond the currently available computing power. Alternative methods, which solve the Boltzmann or model equations directly with the discretization of the phase space [3, 18], have attracted attentions in recent years.

Among continuum solution methodologies, there are primarily two approaches: (1) the Chapman-Enskog method [9], and (2) the method of moments [13]. In the Chapman-Enskog method, the phase density is expanded in powers of the Knudsen number, the zeroth-order expansion yielding the Euler equations, the first-order results in the equations of Naver-Stokes and Fourier, the second order the Burnett equations, and the third order expansion the so-called super-Burnett equations. It is well recognized that the equations of Navier-Stokes and Fourier cease to be accurate for Knudsen number above 0.1, and one might theorize that the Burnett and Super-Burnett equations are valid for larger Knudsen numbers. Unfortunately, the higher-order equations are shown to be linearly unstable for processes involving small wavelengths, or high frequencies, and thus cannot be used in numerical simulations [8]. In recent years, several authors presented augmented forms of the Burnett equations containing additional terms of the super-Burnett order as a way of stabilizing the Burnett equations [35], the BGK-Burnett equations [4], or the regularized hyperbolic equations through relaxation, reproducing the Burnett equations when expanded in Kn [16].

In the method of Grad, the Boltzmann equation is replaced by a set of moment equations which are the first order partial differential equations for the moments of the dis-