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Non-Equilibrium Flow Modeling Using High-Order Schemes for the Boltzmann Model Equations

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We consider application of higher-order schemes to the Boltzmann model equations with a goal to develop a deterministic computational approach that is accurate and efficient for simulating flows involving a wide range of Knudsen numbers. The kinetic equations are solved for two non-equilibrium flow problems, namely, the structure of a normal shock wave and an unsteady two-dimensional shock tube. The numerical method comprises the discrete velocity method in the velocity space and the finite volume discretization in physical space with different numerical flux schemes: the first-order, the second-order minmod flux limiter as well as a third-order WENO scheme. The normal shock wave solutions using BGK and ES collision models are compared to the DSMC simulations. The solution for unsteady shock tube is compared to the Navier-Stokes simulations at low Knudsen numbers and the rarefaction effects in such flow are also discussed. It is observed that a higher-order flux scheme provides a better convergence rate and, hence, reduces the computational effort. The entropy generation rate is shown to be a very sensitive indicator of the onset of non-equilibrium as well as accuracy of a numerical scheme and consistency of boundary conditions in both flow problems.

I. Introduction

In regions of non-equilibrium, which are encountered frequently in supersonic flows at high altitudes and flows expanding into vacuum, the macroscopic conservation laws based on the continuum hypothesis tend to breakdown. The limits on the conventional mathematical models can be understood in terms of the Knudsen number ($Kn = \frac{\lambda}{L}$) where λ is the average distance traveled by the molecules between collisions, or mean free path, and L is the characteristic length scale. When the flow gradients are large, the scale length is of the same order as the mean free path and the transport terms in continuum equations fail. When the continuum equations break down, as in the case of a flow within a normal shock wave and many other flow conditions, a model at the molecular level is required. One approach is to directly simulate the random motion of particles using the Direct Simulation Monte Carlo (DSMC). However, the DSMC method, which allows for non-equilibrium physics, requires high computation power. The mathematical model which describes the motion of molecules is the Boltzmann equation. However, due to it's complex non-linearity, obtaining an analytical solution is not possible for non-trivial problems. Moreover, it presents numerous difficulties to conventional numerical methods. A one dimensional flow of a monatomic gas becomes a four-dimensional problem in phase space with one spatial dimension and three velocity components. Similarly, a two dimensional flow becomes a five-dimensional problem. As a result, it is of great interest

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