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SHOCK AND BOUNDARY STRUCTURE FORMATION BY SPECTRAL-LAGRANGIAN METHODS FOR THE INHOMOGENEOUS BOLTZMANN TRANSPORT EQUATION*

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Abstract

The numerical approximation of the Spectral-Lagrangian scheme developed by the authors in [30] for a wide range of homogeneous non-linear Boltzmann type equations is extended to the space inhomogeneous case and several shock problems are benchmark. Recognizing that the Boltzmann equation is an important tool in the analysis of formation of shock and boundary layer structures, we present the computational algorithm in Section 3.3 and perform a numerical study case in shock tube geometries well modeled in for $1D$ in $\mathbf{x}$ times $3D$ in $\mathbf{v}$ in Section 4. The classic Riemann problem is numerically analyzed for Knudsen numbers close to continuum. The shock tube problem of Aoki et al [2], where the wall temperature is suddenly increased or decreased, is also studied. We consider the problem of heat transfer between two parallel plates with diffusive boundary conditions for a range of Knudsen numbers from close to continuum to a highly rarefied state. Finally, the classical infinite shock tube problem that generates a non-moving shock wave is studied. The point worth noting in this example is that the flow in the final case turns from a supersonic flow to a subsonic flow across the shock.

Mathematics subject classification: 65T50, 76P05, 76M22, 80A20, 82B30, 82B40, 82B80
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1. Introduction

A gas flow may be modeled on either a microscopic or a macroscopic level. The macroscopic model regards the gas as a continuum and the description is in terms of variations of the macroscopic velocity, density, pressure and temperature with space and time. On the other hand, the microscopic or molecular model recognizes the particulate structure of a gas as a myriad of discrete molecules and ideally provides information on the position and velocity of every molecule at all times. However, a description in such detail is rarely, if ever, practical and a gas flow is almost invariably described in terms of macroscopic quantities. The two models must therefore be distinguished by the approach through which the description is obtained, rather than by the nature of the description itself. This paper is concerned with the microscopic

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approach and the first question which must be answered is whether this approach can solve problems that could not be solved through the conventional continuum approach.

A gas at standard conditions (1 bar, 25^oC) contains ca. 2.43×10^{16} particles per cubic millimeter. Despite this huge number of individual particles, a wide variety of flow and heat transfer problems can be described by a rather low number of partial differential equations, namely the well known equations of Navier-Stokes. Due to the many collisions between particles which effectively distribute disturbances between particles, the particles behave not as individuals, but as a continuum. Under standard conditions, a particle collides with the others very often, about 10^9 times per second, and travels only very short distances between collisions, about 5×10^{-8}m. Both numbers, known as collision frequency ν and mean free path l_0, depend on the number density of the gas.

The macroscopic quantities at any point in a flow may be identified with average values of appropriate molecular quantities; the averages being taken over the molecules in the vicinity of the point. The continuum description is valid as long as the smallest significant volume in the flow contains a sufficient number of molecules to establish meaningful averages. The existence of a formal link between the macroscopic and microscopic quantities means that the equations which express the conservation of mass, momentum and energy in the flow may be derived from either approach. While this might suggest that neither of the approaches can provide information that is not also accessible to the other, it must be remembered that the conservation equations do not form a determinate set unless the shear stresses and heat flux can be expressed in terms of the other macroscopic quantities. It is the failure to meet this requirement, rather than the breakdown of the continuum description, that places a limit on the range of validity of the continuum equations. More specifically, the Navier-Stokes equations of continuum gas dynamics fail when gradients of the macroscopic variables become so steep that their scale length is of the same order as the average distance traveled by the molecules between collisions, or *mean free path*, l_0. A less precise but more convenient parameter is obtained if the scale length of the gradients is replaced by the characteristic dimension of the flow, L_{flow}. Flow problems in which typical length scales L_{flow} are much larger than the mean free path l_0, or in which the typical frequencies ω are much smaller than ν, are well described through the laws of Navier-Stokes. The *Knudsen number* $Kn = l_0/L_{flow}$ is the relevant dimensionless measure to describe these conditions, and the Navier-Stokes equations are valid as long as $Kn \ll 1$.

This condition fails to hold when the relevant length scale L_{flow} becomes comparable to the mean free path l_0. This can happen either when the mean free path becomes large, or when the length L_{flow} becomes small. A typical example of a gas with large mean free path is high altitude flight in the outer atmosphere, where the mean free path must be measured in meters, not nanometers, and the Knudsen number becomes large for, e.g., a spacecraft. Miniaturization, on the other hand, produces smaller and smaller devices, e.g., micro-electro-mechanical systems (MEMS), where the length L_{flow} approaches the mean free path.

Moreover, the Navier-Stokes equations will fail in the description of rapidly changing processes, when the process frequency ω approaches, or exceeds, the collision frequency ν. The Knudsen number ($Kn = \omega/\nu$) is used to classify flow regimes as follows:

- $Kn \ll 1$, i.e., $Kn \precsim 0.01$: The hydrodynamic regime, which is very well described by the Navier-Stokes equations.
- $0.01 \precsim Kn \precsim 0.1$: The slip flow regime, where the Navier-Stokes equations can describe the flow well, but must be supplied with boundary conditions that describe velocity slip and temperature jumps at gas-wall interfaces (rarefaction effects).