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A Direct Solver for Initial Value Problems of Rarefied Gas Flows of Arbitrary Statistics

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Abstract. An accurate and direct algorithm for solving the semiclassical Boltzmann equation with relaxation time approximation in phase space is presented for parallel treatment of rarefied gas flows of particles of three statistics. The discrete ordinate method is first applied to discretize the velocity space of the distribution function to render a set of scalar conservation laws with source term. The high order weighted essentially non-oscillatory scheme is then implemented to capture the time evolution of the discretized velocity distribution function in physical space and time. The method is developed for two space dimensions and implemented on gas particles that obey the Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Computational examples in one- and two-dimensional initial value problems of rarefied gas flows are presented and the results indicating good resolution of the main flow features can be achieved. Flows of wide range of relaxation times and Knudsen numbers covering different flow regimes are computed to validate the robustness of the method. The recovery of quantum statistics to the classical limit is also tested for small fugacity values.

AMS subject classifications: 82-08, 82B30, 82B40, 35Q20

Key words: Semiclassical Boltzmann-BGK equation, weighted essentially non-oscillatory, discrete ordinate method.

1 Introduction

In kinetic theory of gases, the Boltzmann equation has been widely used to describe various transport phenomena in classical rarefied gas covering wide range of flow param-

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eters such as Reynolds number, Mach number and Knudsen number. The Chapman-Enskog expansion method is usually applied to the Boltzmann equation to derive closed set hydrodynamic transport equations that apply to a broad range of flow regimes, see [8]. In analogy to the classical Boltzmann equation, a semiclassical Boltzmann equation, which generalizes the collision term in order to treat the collision of particles of quantum statistics, has been developed; For detail, readers may refer to [21, 34]. Hydrodynamic behaviour of quantum gases has been the subject of some prominent researches, see [3, 28, 36], and the application of quantum Boltzmann hydrodynamic equations have been implemented in the analysis of electron flows in quantum semiconductor devices, such as in the works of [2, 12, 37]. In recent years, due to the rapid advancements of microtechnology and nanotechnology, the device or structure characteristic length scales become comparable to the mean free path and the wavelength of energy and information carriers (mainly electrons, photons, phonons, and molecules), some of the classical continuum transport laws are no longer applicable. It is generally believed that the microscopic description of Boltzmann equation (classical and semiclassical) is adequate to treat transport phenomena in the mesoscale range. Different types of carriers may involve simultaneously in a single problem, therefore, it is desirable to have a method that can allow one to treat them in a unified and parallel manner. Indeed, this is the view advocated in micro- and nano-scale energy transport by Chen [9]. With the semiclassical Boltzmann equation, it is possible to describe adequately the mesoscale transport of particles of arbitrary statistics.

The principal difficulty encountered in solving semiclassical Boltzmann equation as derived by Uehling and Uhlenbeck is the same as that encountered in the classical counterpart and is mainly due to the complicated integral nature of its collision term. The relaxation time approximation proposed by Bhatnagar, Gross and Krook (BGK) [4] for the classical Boltzmann equation provides a much simpler form of collision term and retains the principal effects of particle collisions and enables more tractable solution methods. The BGK relaxation time concept is rather general and can be applicable to the semiclassical Boltzmann equation as well. The only change is that the equilibrium Maxwell-Boltzmann distribution in the classical case is replaced by the Bose-Einstein or Fermi-Dirac distribution depending on the types of carrier particles. The semiclassical Boltzmann-BGK equation has been widely applied for electron carrier transport in semiconductor [5–7, 11, 25–27, 29, 30] and phonon energy transport in thermoelectric materials [9]. Similarly, the solution methodology developed for classical Boltzmann-BGK equation can be applied to the semiclassical Boltzmann-BGK equation in phase space. In this work, we aim at developing an accurate direct solver for the semiclassical Boltzmann-BGK equation in phase space that can treat particles of three statistics on equal foot and in a parallel manner. Such a method will allow one to examine the same physical flow problems but with different gas of particles. It is noted that even when solving the problems for the classical Maxwell-Boltzmann statistics, the present formulation allows the analysis fugacity which has not been included in the original Boltzmann-BGK equation [4] nor in most of other existing works based on it. First, depending on