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1. Introduction

In recent years, due to the rapid advancements of microtechnology and nanotechnology, the characteristic length scales of the device or structure become comparable to the mean free path and the wavelength of energy and information carriers (mainly electrons, photons, phonons, and molecules), the classical continuum transport laws are no longer applicable.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. Besides, due to the different types of carriers may involve simultaneously in a single problem, it is desirable to have a method that can allow one to treat them in a unified and parallel manner. With the semiclassical Boltzmann equation, it is possible to describe adequately the mesoscale transport of particles of arbitrary statistics. The Bhatnagar-Gross-Krook relaxation time concept \cite{1} can be applicable to gases of particles of general statistics and is adopted in this study. The solution methodology developed in \cite{2} can be applied to the present semiclassical Boltzmann-BGK equation in phase space. In this note, first, the discrete ordinate method is used to discretize the velocity (or momentum or wave number) space in the semiclassical Boltzmann-BGK equation into a set of equations in physical space with source terms that are independent of molecular velocity. Second, the resulting equations can be treated as scalar hyperbolic conservation laws with stiff source terms. Here, an explicit, second-order conservation element and solution element (CE/SE) scheme developed by Chang \cite{3, 4, 5} for solving conservation laws is adopted to describe the evolution of these equations. Due to the complexity of the transport problems of different particle statistics, an accurate yet simple numerical method exempt from the applications of Riemann solvers, flux splittings and monotonicity constraints, all exhibited by CE/SE is desired. The application of CE/SE on systems of distribution functions may exhibit different results when conventional upwind based schemes are applied instead. This is due to its nontraditional features which includes: (i) a unified treatment of space and time; (ii) the introduction of conservation elements (CEs) and solution elements (SEs) as the vehicles for enforcing space-time flux conservation; (iii) exclusion of interpolation nor extrapolation procedure for computation of fluxes at an interface. Our goal is to first develop a 1D solver before considering a multi-dimensional approach. This is due to the demanding computational costs when 2D and 3D solvers are considered. We believe that these findings shall give a strong ground before advancing to multi-dimensional analysis eventually. In this note, numerical experiments of one-dimensional semiclassical gas dynamical flows near low densities are presented to demonstrate the ability of the present algorithm.

2. Semiclassical Boltzmann-BGK Equation

The elements of semiclassical Boltzmann-BGK equation are described as:

\[
\left( \frac{\partial}{\partial t} + \frac{p}{m} \cdot \nabla_x - \nabla U(x, t) \cdot \nabla_p \right) f(p, x, t) = - \frac{f - f^{(0)}}{\tau}
\]  

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where \( m \) is the particle mass, \( U \) is the mean field potential and \( f(\mathbf{p}, \mathbf{x}, t) \) is the distribution function which represents the average density of particles with momentum \( \mathbf{p} \) at the space-time point \( \mathbf{x}, t \). Here, \( \tau \) is the relaxation time and needs to be specified for each carrier scattering. The equilibrium distribution function for general statistics can be expressed as

\[
f^{(0)}(\mathbf{p}, \mathbf{x}, t) = \frac{1}{z^{-1} \exp \left[ [\mathbf{p} - m \mathbf{u}(\mathbf{x}, t)]^2 / 2mk_BT(\mathbf{x}, t) \right] + \theta}
\]  

(2)

where \( \mathbf{u}(\mathbf{x}, t) \) is the mean velocity, \( T(\mathbf{x}, t) \) is temperature, \( k_B \) is the Boltzmann constant and \( z(\mathbf{x}, t) = \exp (\mu(\mathbf{x}, t)/k_B T(\mathbf{x}, t)) \) is the fugacity, where \( \mu \) is the chemical potential. In (2), \( \theta = -1 \) denotes the Fermi-Dirac statistics, \( \theta = +1 \), the Bose-Einstein statistics and \( \theta = 0 \) denotes the Maxwell-Boltzmann statistics. We note that even with the case of \( \theta = 0 \), we still have chemical potential \( \mu \) or fugacity \( z \) which is rather different from the usual classical Maxwellian distribution. The macroscopic dynamic variables of interest such as number density, momentum density and energy density are the first few low order moments of the distribution function and are defined by:

\[
\begin{bmatrix}
  n(\mathbf{x}, t) \\
  j(\mathbf{x}, t) \\
  \epsilon(\mathbf{x}, t)
\end{bmatrix}
= \int \frac{d\mathbf{p}}{h^3} \begin{bmatrix}
  1 \\
  \mathbf{p}/m \\
  \mathbf{p}^2/2m
\end{bmatrix} f(\mathbf{p}, \mathbf{x}, t)
\]  

(3)

where \( h \) is Planck’s constant. Other higher-order moments such as stress tensor \( \mathbf{P}_{ij} \) and the heat flux vector \( \Phi_i(\mathbf{x}, t) \) can also be defined accordingly. The conservation laws of macroscopic properties can be obtained by multiplying Eq. (1) respectively by \( 1 \), \( \mathbf{p} \) and \( \mathbf{p}^2/2m \) and integrating the resulting equations over all \( \mathbf{p} \). Consequently, the integrals of the collision terms in all three cases vanish automatically resulting in the conservation laws in differential equations form for the conserved macroscopic quantities i.e., number density \( n(\mathbf{x}, t) \), momentum density \( \rho \mathbf{u}(\mathbf{x}, t) \), and energy density \( \epsilon(\mathbf{x}, t) \) as follow:

\[
\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_j} (n \mathbf{u}_j) = 0,
\]  

(4)

\[
\frac{\partial \rho \mathbf{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho \mathbf{u}_i \mathbf{u}_j + \Phi_j) = -\rho \mathbf{u} \cdot \nabla \mathbf{u},
\]  

(5)

\[
\frac{\partial \epsilon}{\partial t} + \frac{\partial}{\partial x_j} (\rho \mathbf{u} \cdot \mathbf{u}_j + \Phi_j) = -\rho \mathbf{u} \cdot \nabla U,
\]  

(6)

The transport coefficients such as viscosity \( \eta \) and thermal conductivity \( \kappa \) can be derived in terms of the relaxation time as

\[
\eta = \frac{\tau nk_BT^2 Q_{1/2}(z)}{2Q_{3/2}(z)},
\]  

(7)

\[
\kappa = \frac{\tau nk_BT^2 Q_{1/2}(z)}{2Q_{3/2}(z)} - \frac{\tau nk_BT^2 Q_{1/2}(z)}{2Q_{3/2}(z)},
\]  

(8)

where \( Q_{\nu}(z) \) is the Fermi or Bose function of order \( \nu \) given below. In the following, we will also consider the case of semiclassical Euler limit in which the particle distribution function is always in equilibrium, i.e., \( f = f^{(0)} \) and the collision term of Eq. (1) vanishes automatically. In recent years, kinetic numerical methods for solving the ideal quantum gas flows based on \( f = f^{(0)} \) have been developed, see [6, 7]. Before we proceed, without losing generality, we neglect the influence of externally applied field \( U(\mathbf{x}, t) \). To illustrate the present method, we formulate the general distribution in one spatial dimension as the following.

\[
f(p_x, x, t) = \frac{1}{z^{-1} \exp \left[ (p_x - mu_x)^2 / 2mk_BT(x, t) \right] + \theta}
\]  

(9)

In a closed form in terms of quantum function, the macroscopic moments, i.e., number density \( n(x, t) \), momentum \( j(x, t) \), energy density \( \epsilon(x, t) \), and pressure \( P(x, t) \) are given by

\[
n(x, t) = \int \frac{dp_x}{h} f^{(0)}(p_x, x, t) = \frac{Q_{1/2}(z)}{A}
\]  

(10)
\[ j(x,t) = \int \frac{dp_x}{h} p_x f_\alpha(0)(p_x,x,t) = n(x,t) u_\alpha(x,t) \]  
(11)
\[ e(x,t) = \int \frac{dp_x}{h} p_x^2 f_\alpha(0)(p_x,x,t) = \frac{Q_{\alpha/2}(z)}{2\beta \lambda} + \frac{1}{2} \nu n u_x^2 \]  
(12)
\[ P(x,t) = nk_BT(x,t) \frac{Q_{\alpha/2}(z)}{Q_{\alpha/2}(\alpha)} \]  
(13)

where \( \lambda = \sqrt{\frac{m \beta}{2k_B T}} \) is the thermal wavelength and \( \beta = 1/k_BT(x,t) \). The functions \( Q_{\alpha}(z) \) of order \( \nu \) are respectively defined for Fermi-Dirac and Bose-Einstein statistics as

\[ \mathcal{F}_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty dx \frac{x^{\nu-1}}{z^{-1} e^x + 1} \approx \sum_{i=1}^\infty (-1)^{i-1} \frac{z^i}{\nu^i} \]  
(14)
\[ \mathcal{B}_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty dx \frac{x^{\nu-1}}{z^{-1} e^x - 1} \approx \sum_{i=1}^\infty \frac{z^i}{\nu^i} \]  
(15)

Here, \( \mathcal{F}_\nu(z) \) applies for Fermi-Dirac integral and \( \mathcal{B}_\nu(z) \) for Bose-Einstein’s, whereas \( \Gamma(\nu) \) is gamma function. The definition of macroscopic quantities in terms of Fermi or Bose function applies for both cases of quantum distributions. Before proceeding to the analysis of the integrals, we introduce the characteristic quantities of \( V_\infty \) and \( t_\infty \) for the purpose of normalization. The characteristic velocity and time can be defined as,

\[ V_\infty = \sqrt{\frac{2k_BT_\infty}{m}}, \quad t_\infty = \frac{L}{V_\infty} \]  
(16)

with \( L \) defined as characteristic length of the problem. The normalized semiclassical Boltzmann-BGK equation,

\[ \frac{\partial f(\hat{\nu}_s,\hat{x},\hat{t})}{\partial \hat{t}} + \hat{\nu}_s \frac{\partial f(\hat{\nu}_s,\hat{x},\hat{t})}{\partial \hat{x}} = -\frac{\hat{\nu}_s - f_\alpha(0)}{\tau} \]  
(17)

with particle velocity \( \nu_s \). From this part, our formulations are all considered normalized and the ‘hat’ sign is omitted for simplicity.

### 3. Application of Discrete Ordinate Method

By applying the discrete ordinate method to Eq. (17), the quantum velocity distribution function in phase space \( f(x,v_\sigma,t) \) can be rendered into a set of hyperbolic conservation equation with source terms in a physical space for \( f_\sigma(x,t) \) where \( \sigma = 1, \ldots, N \). The resulting equations are,

\[ \frac{\partial f_\sigma(x,t)}{\partial t} + \nu_\sigma \frac{\partial f_\sigma(x,t)}{\partial x} = -\frac{f_\sigma - f_\sigma(0)}{\tau} \]  
(18)

with \( f_\sigma \) and \( \nu_\sigma \) represent the values of respectively \( f \) and \( v_\sigma \) evaluated at the discrete velocity points \( \sigma \). Once we have solved the discrete distribution function \( f_\sigma(x,t) \), then the quadrature method is applied to calculate the macroscopic quantities. In this work, Newton-Cotes formula with adjustable intervals is utilized to cover wide range of velocity. We employ a variant of Newton-Cotes formula i.e., the composite five-point Boole’s rule, see [8],[9] and [10]. The repeated Newton-Cotes formula over an interval \( [v_1, v_N] \) divided into \( N \) panels of width \( h = (v_N - v_1)/N \) is

\[ \int_{v_1}^{v_N} f(v) dv = \frac{2}{45} h[7f_1 + 32f_2 + 12f_3 + 32f_4 + 14f_5 \ldots + 32f_{N-1} + 7f_N] - \frac{2(v_N - v_1)M'(6)}{945} h^6, \]  
(19)

where,

\[ M'(6) = \sup_{s\in[v_1,v_N]} \left| f'(6)(s) \right|. \]  
(20)
Here, \( f^{(i)} \) denotes the \( i \)th order derivative.

For every time level we can acquire and update the macroscopic moments in the physical space using a selected quadrature method e.g.,

\[
n(x,t) = \int_{-\infty}^{\infty} f(\upsilon,x,t) d\upsilon \approx h \sum_{\sigma=1}^{N} H_{\sigma} f(\sigma,x,t).
\]  

(21)

4. Numerical Method

A space-time conservation element and solution element \( c - \tau_{c} \) method with extended wiggle suppressing terms (known also as \( w - \alpha \) scheme) is introduced to solve the scalar conservation law with stiff source terms. The requirement of marching variables for 1 time level using CE/SE is divided into two half time steps. To be consisted with the notation with the original work the time integration is carried out from \((n - 1/2)\)th to \(n\)th time level, and subsequently from \(n\)th to \((n + 1/2)\)th time level. The scheme used in this work is \( w - \alpha \) scheme which can be written as

\[
f_{\sigma j}^{n} = \frac{1}{2} [(1 + \nu)f_{\sigma j-1/2}^{n-1/2} + (1 - \nu)f_{\sigma j+1/2}^{n-1/2} + \\
(1 - \nu^{2})[(f_{\sigma j}^{n-1/2} - (f_{\sigma j}^{n-1/2})_{1}) + \\
\Delta t \left( -\frac{f_{\sigma j-1}^{n} - f_{\sigma j}^{n-1}}{\tau} \right)].
\] 

(22)

where

\[
(f_{\sigma j})^{0}_{j} = f_{\sigma j-1/2}^{(n-1/2)} + (w_{j})^{0}_{j}(f_{\sigma j-1}^{0})_{j}^{n}
\]

(23)

with the weighting functions \((w\pm)^{0}_{j}\) defined as

\[
(w\pm)^{0}_{j} = W_{\pm}(f_{\sigma j-1}^{0}, (f_{\sigma j-1/2}^{0})_{j}; \alpha).
\] 

(24)

The parameter \( \tau_{c} \) and \( \alpha \) are chosen constants. In details, the step-by-step algorithm is explained as follow,

1. Initial information of \( f_{\sigma j}^{(n-1/2)} \) and \( f_{\sigma j}^{(n-1)} \), \( \forall j \in \Omega \) are defined. \( \Omega \) denote the set of all staggered space-time mesh points \((j, n)\) in an Euclidian space \( E_{2} \). For every \( j \in \Omega \), the normalized term \( f_{\sigma j}^{(n-1/2)} \) can be calculated from \( f_{\sigma j}^{(n-1/2)} \) using the relation \((f_{\sigma j})^{0}_{j} = (\Delta x/4)(f_{\sigma j})^{n}_{j} \). At this initial state, the equilibrium values, \( f_{\sigma j}^{(n-1/2)} \) is defined the same as \( f_{\sigma j}^{(n-1/2)} \). Note that at \((n - 1/2)\)th, \( j \notin \Omega \) if \((j, n) \in \Omega \) (see Fig. 2(a)).

2. After initialization in step 1, \( f_{\sigma j}^{n} \), \( \forall j \in \Omega \), can be calculated using Eq. (22).

3. Eq. (23) is employed along with Eq. (24) to acquire the second marching variable \( f_{\sigma j}^{n+1/2} \), i.e., \( f_{\sigma j}^{(n+1/2)} \), \( f_{\sigma j}^{n+1} \) (calculated in step 2) and \( f_{\sigma j}^{n} \), \( \forall j \in \Omega \) are variables required in order to advance to \((n + 1/2)\)th time level.

4. Step 2 shall be repeated to reach \((n + 1/2)\)th time level from \(n\)th time level. For example, when calculating \( f_{\sigma j+1/2}^{n+1} \), Eq. (22) will be applied by shifting \( n \rightarrow (n + 1/2) \) and \( j \rightarrow (j + 1/2) \) to obtain

\[
f_{\sigma j+1/2}^{n+1} = \frac{1}{2} [(1 + \nu)f_{\sigma j}^{n+1} + (1 - \nu)f_{\sigma j+1}^{n+1} + \\
(1 - \nu^{2})[(f_{\sigma j}^{n+1/2} - (f_{\sigma j}^{n+1/2})_{1}) + \\
\Delta t \left( -\frac{f_{\sigma j+1}^{n+1/2} - f_{\sigma j}^{n+1/2}}{\tau} \right)].
\] 

(26)
Step 3 is repeated; Eqs. (23) and (24) are employed (by shifting $n \rightarrow (n + 1)/2$ and $j \rightarrow (j + 1)/2$) to calculate
\[
(f_{xj}^{n+1/2})
\]
At this stage we have completed the integration of Eq. (18) for one full time step. The whole procedure shall be repeated to obtain the next time level. To be consistent with the molecular collision theory, the time step size ($\Delta t$) has to be less than the local mean collision time $\tau$. After acquiring the macroscopic moments from Eqs. (10), (11) and (12), we need to use the combination of these equations to update the values of $z(x, t)$ and $T(x, t)$. To solve $z(x, t)$, which is the root of equation
\[
\Psi_1(z) = \epsilon - \frac{Q_{1/2}}{4\pi} \left( \frac{n}{Q_{1/2}} \right)^3 - \frac{1}{2} nu^2_z
\]
(27)

5. Computational Results

We chose to solve the one-dimensional gas flow problems near low densities. This problem was first proposed in [11] and is chosen for demonstrating the ability of the method to preserve the positivity of density and internal energy. In this problem a diaphragm is located at $x = 0.5$, separating two regions of gases of arbitrary statistics; each remains in a constant equilibrium state at initial time $t = 0$. The macroscopic properties on both sides of the diaphragm are set different and given with $(z, U, T) = (0.446, -2, 1.6)$ for $0 \leq x \leq 0.5$ and $(z, U, T) = (0.446, 2, 1.6)$ for $0.5 \leq x \leq 1$. As the diaphragm is released, strong rarefaction waves propagate toward opposite directions. In Fig. 1, the plots of density, pressure, energy, fugacity, temperature and velocity are given for the three statistics. The given initial condition correspond to different values of densities, pressures and energies for the three statistics as can be seen in the figure. In this example, 300 grid points are used with 800 Newton-Cotes discrete velocity points. $\tau = 0.001$ is used with Courant number of 0.1. CE/SE scheme with $\alpha = 3$ is utilized. In Fig. 2, the range of constant relaxation times are tested to test the robustness of the algorithm. For the case of Maxwell-Boltzmann gas, we tested the values of $\tau = 0.001, 0.01, 0.1$ as well as the case of $f = f^{(0)}$ by which the solution shall be regarded as that of Euler solution. In this example 400 grid points are used with 900 Newton-Cotes discrete velocity points. For the case of Maxwell-Boltzmann statistic, the given initial condition correspond to $n = 1$ and $P = 0.4$ for $0 \leq x \leq 1$. The results for Maxwell-Boltzmann gas in Euler limit can be compared with the existing works, see [11, 12]. Note that with the current method it is possible to plot fugacity for Maxwell-Boltzmann gas.

6. Concluding Remarks

A direct algorithm constructed to solve semiclassical Boltzmann-BGK equation for particles of all statistics is applied on a one-dimensional gas flow problems utilizing the application of CE/SE scheme. When Fermi-Dirac or Bose-Einstein statistics are considered, we do not have experimental nor computational results yet to compare our results to, especially at transitional regions. However, there are adequate results to compare to when Maxwell-Boltzmann statistic is considered, especially at Euler limit. Therefore quantitative comparisons can possibly be made. Taking into account that all the statistics are treated on an equal foot and on parallel manner, we could be at least assured that the current method and the generated results has sound theoretical ground. Note that CE/SE scheme is formed by two coupled discrete equations (i.e., Eqs (22) and (23)) involving independent numerical variables $f$ and $\partial f/\partial x$; Therefore, when multidimensional case and complex boundary condition e.g., including wall reflection are considered, special treatment at the boundary has to be done in order to maintain a sound physics. This treatment might be unique in regard to the application of CE/SE scheme. Outside the scope of this note, the extension to multi-dimensional cases covering more complex geometries with boundary value problems using CE/SE will be subject to a further study.

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References


Figure 1: Macroscopic properties of Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein gases
Figure 2: Macroscopic properties of Maxwell-Boltzmann gases at $\tau = 0.1, 0.01, 0.001$ and the Euler solution.