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On the time relaxed Monte Carlo computations for the flow over a flat nano-plate

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ABSTRACT

In the present study, the first, second and third orders of the TRMC scheme (TRMC1, TRMC2 and TRMC3 schemes) are employed to numerically investigate the Argon flow over a flat nano-plate with different free stream velocities and variety of Knudsen numbers. The simulations cover flow regimes from early slip to early transition regimes ($0.00129 \leq Kn \leq 0.09$). Higher order terms in the Wild sum expansion are considered to obtain higher order collisions. The results are compared with those from the standard DSMC method. Comparisons show that among the studied schemes, the results obtained from the TRMC3 scheme have excellent agreement with the ones from the DSMC method. On the other hand, the results of the TRMC1 and TRMC2 schemes show deviations compared to those from the DSMC method. The deviations are more pronounced for the temperature and pressure distributions. Moreover, the present investigation illustrates that as the Knudsen number increases the accuracy of lower orders of the TRMC scheme improves. It is observed that truncating the Wild sum expansion up to the third order approximation of the TRMC scheme, may be a proper alternative method for the DSMC method in simulating the flow over the nano-plate for Knudsen numbers $0.00129 \leq Kn \leq 0.09$ with reasonable accuracy and simplicity in mathematics.

1. Introduction

Navier–Stokes equations lose the capability of simulating the flow accurately, when the characteristic length of the flow is comparable to the mean free path. For such flows, the governing equation is the Boltzmann equation of kinetic theory [1,2]. During the past decades, the direct simulation Monte Carlo (DSMC) method has been extensively adopted for the numerical solution of the Boltzmann equation in rarefied regimes [1–3]. Despite the simplicity and reasonable accuracy of the DSMC method, high computational expenses of the flow simulations is the main concern. The computational expenses of the DSMC method drastically increase as the Knudsen number decreases, where the expenses of the DSMC method cannot be justified for the flows near the continuum region. Hence, introducing schemes to reduce the computational expenses of numerical solution of the Boltzmann equation, are highly interested [3–7]. Recently, the time relaxed Monte Carlo (TRMC) method has been introduced as a simple and efficient method to numerically solve the Boltzmann equation in the flows with wide variation of Knudsen numbers. In the algorithm of the TRMC scheme, time discretizations are obtained from the Wild [8] sum expansion with the higher order collisions being replaced by the local Maxwellian distribution [9].

It is illustrated that the TRMC method performs in the same way as the standard DSMC method for large Knudsen numbers, while local Maxwellian distribution replaces the time consuming collision calculations, as the Knudsen number decreases. Furthermore, the capability of adopting larger time steps compared to the ones in the DSMC method is another advantages of the TRMC scheme over the standard DSMC method [3]. On the other hand, complexity of the TRMC scheme, especially for higher order schemes, is the main drawback of the scheme. Pareschi and Russo [10] performed the stability analysis on the TRMC scheme and proved the A-stability and L-stability of the scheme. Moreover, using the TRMC scheme they obtained reasonable solution of the Kac equation compared to the results from standard DSMC method. Furthermore, Pareschi et al. [11–13] introduced algorithm for the TRMC scheme using the variable hard sphere model for inter-molecular collisions. They also studied one-dimensional shock wave problem and obtained reasonable results compared to the ones from the standard DSMC method. Pareschi and Trazzi [3] presented algorithms to obtain the first and second orders of the TRMC scheme that simultaneously preserve the conserva-

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Nomenclature

μ	the mean collision frequency, kinematic viscosity
ρ	density
τ	relaxed time, shear stress
F	transformed probability distribution function
f	probability distribution function
Kn	Knudsen number
L	characteristic length
M	local Maxwellian distribution
P	collisional operator, pressure
Q	collisional operator
T	temperature
t	time
U	velocity
υ	velocity vector

Subscripts

∞	free stream condition
mps	most probable molecular thermal speed
x, y	x and y directions, respectively

tion of mass, momentum, and energy. They also simulated the gas flow around an obstacle using the TRMC method and obtained an appreciable reduction in the CPU time, compared to that from the standard DSMC method. Foreseeing higher accuracies, Russo et al. [14] introduced the third order TRMC scheme by considering higher order collisions in truncating the Wild sum expansion. They performed the TRMC and DSMC methods to investigate the Couette flow for a wide variety of Knudsen numbers and several wall velocities. The comparisons indicated that the density, velocity and temperature profiles, obtained from the TRMC scheme, are in excellent agreement with the ones from the DSMC method. Moreover, Ganjaei and Nourazar [15] studied Argon and Helium mixture flow inside a rotating cylinder using the TRMC and DSMC methods. They used Dalton's law for partial pressures of each species and showed that the results of TRMC method are in excellent agreement with the analytical solution. They reached more accurate results using the TRMC scheme, compared to the results from standard DSMC scheme. Trazzi et al. [16] introduced the recursive TRMC scheme to obtain uniform accuracy in time, independent of time step. They obtained considerable improvement in the computational efficiency of simulating the space homogeneous test cases and non-homogeneous stationary shock problem, in comparison to the standard DSMC method. Most recently, Dimarco and Parechi [17] decomposed the collision operator of the Boltzmann equation into an equilibrium and a non-equilibrium parts and introduced the exponential Runge–Kutta scheme. They performed the first and second orders of integrating factor (IF) scheme to study the heat flux in a space homogeneous shock wave problem. They obtained results with excellent agreement with the ones from the standard DSMC method for $Kn = 0.001$, while both the first and second orders of IF scheme showed significant error for the flow with $Kn = 0.0001$. Furthermore, Eskandari and Nourazar [18] performed the first, second and third orders of the TRMC scheme to study a lid-driven micro cavity flow with different lid velocities and Knudsen numbers. They obtained results with excellent agreement with the ones from the standard DSMC method, using the third order time relaxed Monte Carlo (TRMC3) scheme.

1.1. The purpose of the present work

The present work focuses on investigating the truncation effects of the Wild sum expansion on the accuracy of the TRMC scheme. Three orders of the TRMC scheme called TRMC1, TRMC2 and TRMC3 schemes are considered accordingly. Argon flow over a flat nano-plate with different free stream velocities and several Knudsen numbers is considered as the benchmark problem. The Knudsen numbers cover flows from early slip to early transition regimes ($0.00129 \le Kn \le 0.09$). The obtained results are compared with the ones either from the standard DSMC method or the results reported from the hybrid DSMC-NS scheme [19].

2. Mathematical description

2.1. The Boltzmann equation

The Boltzmann equation for a single component mono-atomic dilute gas in the absence of external forces, is described by the following equation, where the bilinear operator $Q(f, f)$ describes the intermolecular collisions [1,2]:

$$\frac{\partial f}{\partial t} + \upsilon \cdot \nabla_x f = \frac{1}{Kn} Q(f, f). \tag{1}$$

Considering $Q(f, f) = P(f, f) - \mu f$, the Boltzmann equation takes the form below [5,8,20]:

$$\frac{\partial f}{\partial t} + \upsilon \cdot \nabla_x f = \frac{1}{Kn} (P(f, f) - \mu f). \tag{2}$$

$P(f, f)$ is a symmetric bilinear operator describing the collision effects of the molecules and the parameter $\mu \neq 0$ is the mean collision frequency. It is common to split the Boltzmann Eq: (2) into the equation of pure convection step (i.e. $Q(f, f) \equiv 0$) (3) and the equation of collision step (i.e. $\upsilon \cdot \nabla_x f \equiv 0$) (4) [1,3,9,16,21].

$$\frac{\partial f}{\partial t} + \upsilon \cdot \nabla_x f = 0. \tag{3}$$

$$\frac{\partial f}{\partial t} = \frac{1}{Kn} (P(f, f) - \mu f). \tag{4}$$

The equation of convection step (3) can be directly solved leaving only concerns about the equation of collision step (4).

2.2. The DSMC approach

The DSMC approach is simply obtained by applying the Euler upwind scheme to the equation of collision step (4):

$$f^{n+1} = \left(1 - \frac{\mu \Delta t}{Kn}\right) f^n + \left(\frac{\mu \Delta t}{Kn}\right) \frac{P(f, f)}{\mu}. \tag{5}$$

Mathematical equation of the DSMC method (5) can be probabilistically interpreted in the following way:

In order to sample a particle from f^{n+1}, it shall be sampled from f^n with probability of $(1 - \mu \Delta t/Kn)$ and shall be sampled from $P(f, f)/\mu$ with probability of $\mu \Delta t/Kn$. Since probability of event can accept neither negative values nor values larger than unity, the time step in the DSMC method shall be selected with the following consideration: $0 \le (\mu \Delta t/Kn) \le 1$ [3].

2.3. The TRMC approach

The relaxed time τ and the transformed probability distribution function $F(\upsilon, \tau)$ are described as the followings [3,9]:

$$\tau = (1 - e^{-\mu t/Kn}). \tag{6}$$

$$F(\upsilon, \tau) = f(\upsilon, \tau) e^{-\mu t/Kn}. \tag{7}$$