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A novel algorithm for implementing a specified wall heat flux in DSMC: Application to micro/nano flows and hypersonic flows

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ABSTRACT

This paper introduces a modified version of the iterative (IT) technique called the modified iterative (MIT) technique which implements a desired wall heat flux distribution over the wall for rarefied gas simulations using the direct simulation Monte Carlo (DSMC) method. The accuracy of the MIT technique and suitable ranges of employed parameters are examined in various test cases, i.e., shear driven Couette and cavity flows, hypersonic/supersonic flows over flat plate/cylinder, and pressure-/inertia-driven flows through micro/nanochannel. In each simulated test case, rarefied gas is considered in the presence of the wall with the specified heat flux distribution. We show that the controlling factor is a critical parameter that adjusts the speed of wall temperature update. This parameter should be selected appropriately for faster solution convergence. Additional considerations in the MIT technique are also presented and investigated. The possibility of employing an efficient hybrid approach based on MIT and inverse temperature sampling (ITS) techniques for implementing the specified wall heat flux is also examined.

1. Introduction

Rarefied gas dynamics is a diverse field, encompassing, for example, high altitude hypersonic flow fields, the reflective and reactive characteristics of gases interacting with solid and liquid surfaces, energy transfer phenomena in molecular collisions, aerosol dynamics, cluster formation and topology, flows induced by evaporation and condensation, upper-atmospheric dynamics, and the attainment of milli-Kelvin temperatures by flow cooling techniques [1]. In rarefied gas flows, the molecular mean free path (λ) is comparable with respect to the length scale of flow properties changes (L). In such flows, analysis must be performed using accurate approaches based on the solution of the Boltzmann equation [2].

In many of above mentioned flows, gas-surface heat transfer plays an essential role in flow field properties. For this reason, developing computational tools for simulation of rarefied gas flows under controlled gas-surface heat exchange is crucial for the study of flow physics and thermal engineering applications. There are several techniques for implementation of specified wall heat flux in rarefied gas flows using analytical, molecular, and continuum-based approaches [3–19]. In some rarefied gas simulations [20–22], adiabatic wall condition have been performed by employing equal temperatures for gas and surface, especially for low-speed flows. It is a simple way for simulation of adiabatic wall condition in low-speed flows. This adiabatic wall condition could be named as both uniform wall temperature (UWT) as well as uniform wall heat flux (UWH) conditions. There are numbers of publications, for example [3–5], which implement specified wall heat flux in analytical and continuum-based approaches using adjusting the temperature gradient near the wall:

$$q_w = -k \left.\frac{\partial T}{\partial n}\right|_{n=0}, \tag{1}$$

where k is the conductivity and n is the direction normal to the wall. Using Eq. (1) and temperature jump condition, wall temperature is obtained. Temperature jump condition is used for slip flow modeling in analytical, and continuum-based analyzes of rarefied gas flow [5]:

$$T_w = T|_{n=0} - \left[\alpha\lambda \frac{\partial T}{\partial n} - \beta\lambda^2 \frac{\partial^2 T}{\partial n^2}\right]_{n=0}, \tag{2}$$

where λ is the local mean free path and α, β correspond to first-order and second-order slip models, respectively. Temperature profile adjacent to the wall can be solved analytically or numerically. Then, wall temperature is obtained from the implemented wall heat flux.

Continuum-based approaches are valid for slip and early transitional flow regimes [23,24]. At highly rarefied conditions,

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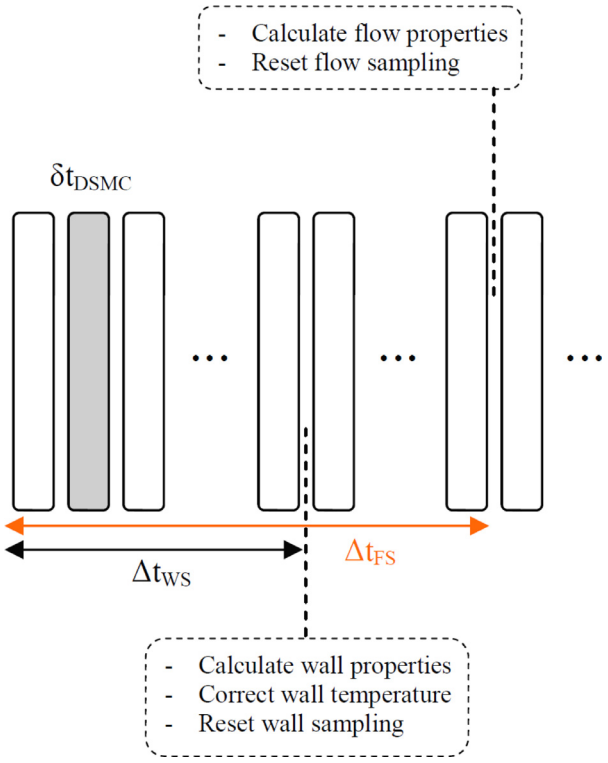

Fig. 1. Sampling processes for flow and wall properties before convergence.

molecular methods are employed for a description of flow fields instead of continuum-based ones. In molecular dynamic (MD) simulations [6–11], the heat flux in a periodic region could be created by exchanging velocities of the particles in "cold" and "hot" slabs located in the middle of the simulation box and adjacent to one of the simulation box boundaries. This exchange periodically results in the heating up of the hot slab and cooling down of the cold slab and finally leads to a steady-state temperature gradient due to thermal conduction through slabs [7]. The imposed heat flux is as:

$$\langle J(t)\rangle = \sum_{\text{transfers}} \frac{m}{2}\left(v_c^2 - v_h^2\right), \tag{3}$$

Table 1
Reference values employed in the MIT technique for various simulation cases.

Simulation test case	ρ_o	T_o	U_o
Couette	ρ_{bulk}	T_{wall}	U_{wall}
Flat plate	ρ_∞	T_∞	U_∞
Pressure-driven	ρ_{in}	T_{in}	U_{in}
Inertia-driven	ρ_{in}	T_{in}	U_{in}
Cavity	ρ_{avg}	T_{lid}	U_{lid}
Cylinder	ρ_∞	T_∞	U_∞

where v_c and v_h are the velocities of particles correspond to cold and hot slabs. The new and old velocities after and before the exchange are related according to [8]:

$$v_c^{new} = v_h^{old}$$
$$v_h^{new} = v_c^{old} \tag{4}$$

There are several published papers that present numerical techniques for implementation of wall heat flux in the direct simulation Monte Carlo (DSMC) method [12–17,19]. Genovesi [12] implemented an adiabatic viscous wall by taking the magnitude of the particle speed as a constant through a collision with the wall. A uniform distribution was assigned for the direction of reflected particles. Wang et al. [13–15] introduced an inverse temperature sampling (ITS) technique to implement specified wall heat flux (SWH) boundary condition in the DSMC method. In the ITS technique, the local wall temperature is obtained from the local specified gas-surface heat exchange ($\Delta\varepsilon$) as:

$$T_w = \frac{\varepsilon^{inc} - \Delta\varepsilon}{\kappa(4+\zeta_{rot})/2}, \tag{5}$$

where κ and ζ_{rot} correspond to the incident energy flux, Boltzmann constant, and number of rotational degrees of freedom, respectively. Their results showed that the ITS technique would be able to impose the specified heat flux rate distribution correctly at the wall. ITS technique also was modified for multi-atomic gasses [15]. Inappropriate initial wall temperature distribution or severe cooling condition may lead to negative unphysical wall temperature values during the simulation [17]. Tzeng et al. [16] presented a wall-fluid molecule collision rule for the description of an adiabatic solid-wall boundary condition in atomistic simulations of rarefied gas natural convection. In this method, the magnitude of the particle velocity is kept invariant before and after the collision. The normal velocity component is reversed with the same magnitude

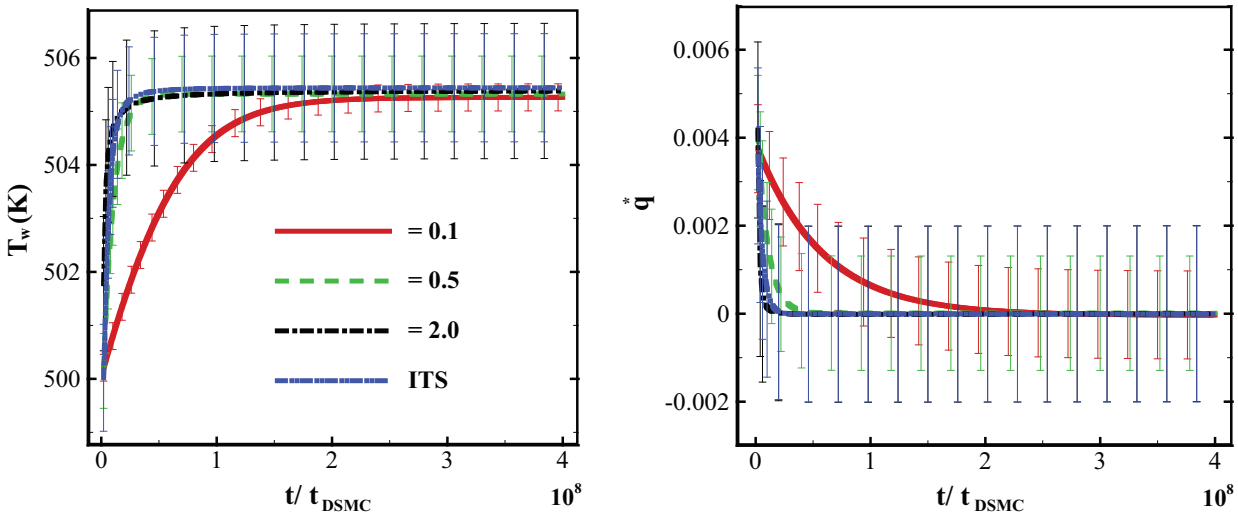

Fig. 2. Comparison of convergence speed for MIT and ITS techniques.