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An Efficient Hybrid DSMC/MD Algorithm for Accurate Modeling of Micro Gas Flows

Tengfei Liang[1] and Wenjing Ye[1,2,*]

[1] *Department of Mechanical Engineering, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*
[2] *KAUST-HKUST Micro/Nanofluidic Joint Laboratory, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*

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Abstract. Aiming at simulating micro gas flows with accurate boundary conditions, an efficient hybrid algorithm is developed by combining the molecular dynamics (MD) method with the direct simulation Monte Carlo (DSMC) method. The efficiency comes from the fact that the MD method is applied only within the gas-wall interaction layer, characterized by the cut-off distance of the gas-solid interaction potential, to resolve accurately the gas-wall interaction process, while the DSMC method is employed in the remaining portion of the flow field to efficiently simulate rarefied gas transport outside the gas-wall interaction layer. A unique feature about the present scheme is that the coupling between the two methods is realized by matching the molecular velocity distribution function at the DSMC/MD interface, hence there is no need for one-to-one mapping between a MD gas molecule and a DSMC simulation particle. Further improvement in efficiency is achieved by taking advantage of gas rarefaction inside the gas-wall interaction layer and by employing the "smart-wall model" proposed by Barisik *et al*. The developed hybrid algorithm is validated on two classical benchmarks namely 1-D Fourier thermal problem and Couette shear flow problem. Both the accuracy and efficiency of the hybrid algorithm are discussed. As an application, the hybrid algorithm is employed to simulate thermal transpiration coefficient in the free-molecule regime for a system with atomically smooth surface. Result is utilized to validate the coefficients calculated from the pure DSMC simulation with Maxwell and Cercignani-Lampis gas-wall interaction models.

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*Corresponding author. *Email addresses:* tfliang@ust.hk (T. Liang), mewye@ust.hk (W. Ye)

1 Introduction

Gas flows are frequently encountered and utilized in microelectromechanical (MEMS) systems, for example, the pressure gas flows in micro channels and flows surrounding micro resonators and the heated micro plate in Pirani sensors. Gas transport and its interaction with the devices play important roles in device operation and accurate modeling of gas flows is crucial to the design of high-performance MEMS devices [1]. One distinct feature of micro gas flows is the rarefaction caused by the small characteristic size and/or the low ambient pressure. In addition, the large surface-to-volume ratio of MEMS devices dictates a surface-dominant transport. As is well known, Navier-Stokes equations and the no-slip boundary model become increasingly inaccurate as the rarefaction level increases. Alternative approaches are therefore adopted for the modeling of rarefied gas.

There have been numerous approaches developed for the modeling of micro gas flows. Examples include but are not limited to the direct simulation of Boltzmann equation [2–4], kinetic schemes [5,6], physical simulation methods such as molecular dynamics (MD) [7] and the direct simulation Monte Carlo (DSMC) [8]. A common key ingredient in all these approaches is a proper boundary model describing correctly the gas-wall interaction process. Other than the MD approach, almost all other methods employ a phenomenological model built upon statistically averaged particle flux distribution. Currently the two most popular models are Maxwell model [9] and Cercignani-Lampis (CL) model [10]. Despite numerous successful applications of these models particularly in the modeling of high-speed rarefied gas transport, the empirical nature and the need of several parameters denoted as the accommodation coefficients demand a careful assessment of the models and a method to determine the accommodation coefficients for applications related to micro gas flows that are often of low speed. Considerate efforts have been made to experimentally measure the accommodation coefficients in MEMS devices [11,12]. The challenges encountered such as leakage and being prone to temperature variation make it difficult to conduct accurate measurement, which is reflected in part by the discrepancies among the reported values in the literature [13].

The MD method, by tracking the motion of individual molecule, is able to model gas-wall interaction accurately, and has been employed in some cases to validate the empirical models and obtain accommodation coefficients [14–16]. It has been shown that gas-wall scattering process cannot be fully captured by the empirical gas-wall interaction models particularly when the incident gas molecules are at a highly non-equilibrium state [14,16]. A major deficiency of the MD method is its high computational cost. For most micro flow problems, it is impractical to apply the MD method to simulate the entire flow domain. A natural choice is to couple the MD method with other more efficient approaches so that the computationally expensive MD method is applied only in the region where it is needed. The DSMC method is an excellent candidate to be coupled with the MD method. Both approaches are particle based so that the coupling between the two methods is relatively easy to realize. The DSMC, although still computational intensive, is much more efficient than the MD for diluted gas and it has been demonstrated in