Commun. Comput. Phys.
doi: 10.4208/cicp.190912.080213a

Vol. **14**, No. 5, pp. 1147-1173
November 2013

# A Unified Gas-Kinetic Scheme for Continuum and Rarefied Flows III: Microflow Simulations

Juan-Chen Huang[1], Kun Xu[2,*] and Pubing Yu[2]

[1] *Department of Merchant Marine, National Taiwan Ocean University, Keelung 20224, Taiwan.*
[2] *Mathematics Department, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*

Received 19 September 2012; Accepted (in revised version) 8 February 2013

Available online 13 June 2013

**Abstract.** Due to the rapid advances in micro-electro-mechanical systems (MEMS), the study of microflows becomes increasingly important. Currently, the molecular-based simulation techniques are the most reliable methods for rarefied flow computation, even though these methods face statistical scattering problem in the low speed limit. With discretized particle velocity space, a unified gas-kinetic scheme (UGKS) for entire Knudsen number flow has been constructed recently for flow computation. Contrary to the particle-based direct simulation Monte Carlo (DSMC) method, the unified scheme is a partial differential equation-based modeling method, where the statistical noise is totally removed. But, the common point between the DSMC and UGKS is that both methods are constructed through direct modeling in the discretized space. Due to the multiscale modeling in the unified method, i.e., the update of both macroscopic flow variables and microscopic gas distribution function, the conventional constraint of time step being less than the particle collision time in many direct Boltzmann solvers is released here. The numerical tests show that the unified scheme is more efficient than the particle-based methods in the low speed rarefied flow computation. The main purpose of the current study is to validate the accuracy of the unified scheme in the capturing of non-equilibrium flow phenomena. In the continuum and free molecular limits, the gas distribution function used in the unified scheme for the flux evaluation at a cell interface goes to the corresponding Navier-Stokes and free molecular solutions. In the transition regime, the DSMC solution will be used for the validation of UGKS results. This study shows that the unified scheme is indeed a reliable and accurate flow solver for low speed non-equilibrium flows. It not only recovers the DSMC results whenever available, but also provides high resolution results in cases where the DSMC can hardly afford the computational cost. In thermal creep flow simulation, surprising solution, such as the gas flowing from hot to cold regions along the wall

*Corresponding author. *Email addresses:* jchuang@mail.ntou.edu.tw (J.-C. Huang), makxu@ust.hk (K. Xu), mayupb@ust.hk (P. B. Yu)

 

surface, is observed for the first time by the unified scheme, which is confirmed later through intensive DSMC computation.

**PACS**: 51.10.+y, 47.11.-j, 47.11.St, 47.45.-n

**Key words**: Unified scheme, non-equilibrium microflow, thermal creep flows.

## 1 Introduction

The flow regimes are characterized by the Knudsen number $Kn$, which is defined as the ratio of molecular mean free path to a characteristic length scale. The continuum regime is in the range of $Kn < 0.001$, followed by the slip regime $0.001 < Kn < 0.1$. The Knudsen number in the transition regime is between 0.1 and 10. Even though it is commonly believed that the Navier-Stokes equations are applicable in the continuum and slip regimes, the validity of these macroscopic description depends on the physical quantities to be evaluated. Even in a fully continuum flow regime, the Navier-Stokes equations cannot be claimed to describe everything properly, where the ghost effect may appear in some cases [25], especially for those related to heat. Simulation of gas flow around microscale structures becomes important with the rapid development of micro-electro-mechanical systems (MEMS) [15]. As the scale of designed devices goes to $\mu m$ and $nm$ length scale, the use of the formal description of macroscopic equations becomes problematic. Unfortunately, experimental study of microflow is also difficult due to the small physical dimensions. Therefore, the development of accurate numerical algorithm for microflow simulation will play an important role, especially for non-equilibrium flow with heat transfer. The numerical challenge for flow in microdevices is that the flow transport may cover the whole flow regimes, from continuum to free molecular ones.

The direct simulation Monte Carlo (DSMC) method is a particle-based simulation method for rarefied flows [6, 10]. The validity of this method has been presented in an enormous amount of research papers. Due to the particle based nature, the DSMC method cannot effectively reduce the statistical scattering encountered in microscale flows, which presents a very large noise to information ratio for flows having low speed and/or small temperature variation. Since the statistical scattering inherent in DSMC decreases with the inverse square root of the sample size, an extremely large sample size is required to reduce it to a level that is small in comparison with the small macroscopic velocity. This makes DSMC simulation of MEMS flows extremely time-consuming. Many small temperature variation phenomena can be hardly identified. Even with so many limitations in the DSMC method for the microflow computations, the DSMC method is still a reliable and accurate method here. In order to improve its efficiency, many attempts have been tried. One of the attractive scheme is the information preservation (IP) method for low speed rarefied gas flows [14, 20, 26, 40]. Since IP-DSMC updates the macroscopic variables for each DSMC particle, how to evolve the macroscopic variables when two DSMC particles get collision is still an active research topic. Another promising