Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2016-0134

Vol. **22**, No. 2, pp. 338-374
August 2017

A Particle Fokker-Planck Algorithm with Multiscale Temporal Discretization for Rarefied and Continuum Gas Flows

Fei Fei[1,2], Zhaohui Liu[2,*], Jun Zhang[3,4] and Chuguang Zheng[2]

[1] *School of Aerospace Engineering, Huazhong University of Science and Technology, Wuhan 430074, P.R. China.*
[2] *State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huazhong University of Science and Technology, Wuhan 430074, P.R. China.*
[3] *School of Engineering, University of Edinburgh, Edinburgh EH9 3FB, United Kingdom.*
[4] *School of Aeronautic Science and Engineering, Beihang University, Beijing 100191, P.R. China.*

Communicated by Kun Xu

Received 16 August 2016; Accepted (in revised version) 16 January 2017

Abstract. For gas flows with moderate and low Knudsen numbers, pair-wise collisions in the Boltzmann equation can be approximated by the Langevin model corresponding to the Fokker-Planck equation. Using this simplified collision model, particle numerical schemes, e.g. the Fokker-Planck model (FPM) method, can simulate low Knudsen number gas flows more efficient than those based on the Boltzmann equation, such as the Direct Simulation Monte Carlo (DSMC) method. However, as analyzed in this paper, the transport properties of the FPM method deviate from the physical values as the time step increases, and this problem affects its computational accuracy and efficiency for the simulation of multi-scale flows. Here we propose a particle Fokker-Planck algorithm with multiscale temporal discretization (MTD-FPM) to overcome the drawbacks of the original FPM method. In the MTD-FPM method, the molecular motion is tracked following the integration scheme of the Langevin model in analogy to the original FPM method. However, to ensure consistent transport coefficients for arbitrary temporal discretization, a time step dependent friction coefficient has been implemented. Several benchmark problems, including Couette, thermal Couette, Poiseuille, and Sod tube flows, are simulated to validate the proposed MTD-FPM method.

PACS: 47.45.-n, 47.11.St, 51.20.+d

Key words: Particle simulation method, Fokker-Planck model, temporal discretization, multiscale flow.

*Corresponding author. *Email addresses:* ffei@hust.edu.cn (F. Fei), zliu@hust.edu.cn (Z. Liu), jun.zhang@buaa.edu.cn (J. Zhang), cgzheng@hust.edu.cn (C. Zheng)

1 Introduction

Multi-scale gas flows widely exist in the micro-electro-mechanical system (MEMS) and aerospace engineering. One example is the micro-nozzle flow [1, 2], where the gas flow changes from the continuum regime in the gas chamber to the free molecular regime at the exit of the nozzle. Another example is gas flow around reentry vehicle [3, 4], where the flow changes from the free molecule regime to transition regime, and finally enters into the continuum regime as the altitude of vehicle continuously descends. Modeling such multi-scale gas flows is very challenging. In the continuum regime, conventional computational fluid dynamics (CFD) methods based on the Navier-Stokes-Fourier (NSF) equations have been applied successfully. However, the NSF equations are not applicable for gas flows far from equilibrium. On the other hand, gas-kinetic methods based on the Boltzmann equation, such as the DSMC method [5], are efficient in the simulation of rarefied gas flows, but it is too expensive computationally in the continuum regime. Therefore, a numerical method applicable for the whole flow regimes is highly expected.

A straightforward multi-scale method is coupling DSMC method and a CFD scheme directly using domain decomposition, i.e., the DSMC method for the rarefied flow regime and the CFD method for the continuum flow regime, respectively [6–9]. However, DSMC-CFD hybrid approaches suffer from difficulties because of the amalgamation of two fundamentally different types of solvers [10]. It is very critical to transfer information properly at the interface between the DSMC and CFD regions. A better strategy is to develop a unified and unique solver for the whole flow regimes. One big progress in this way is the unified gas-kinetic scheme (UGKS), which was proposed by Xu and Huang [11] and has been successfully applied to a variety of gas flows [12, 13]. Alternatively, our aim is to develop a unified particle simulation method for multi-scale gas flows, since particle method has advantages in adding some physical and chemical models.

Recently, Jenny, Torrilhon, and Heinz [14] have proposed a particle Fokker-Planck model (FPM) method. Then, Gorji et al. further developed the FPM method with correct Prandtl number [15, 16], and applied it to more complex flows (multi-species [17] and diatomic [18]). Different from deterministic numerical approaches [19–21], the particle FPM method solves the Fokker-Planck equation by simulating particle motions. In the rarefied gas regime, previous FPM simulation results have demonstrated that counter Fourier heat fluxes in lid-driven cavity flows of Kn$\approx$0.05 [16] and mass flow rates in Poiseuille flow up to Kn$\approx$5 [15] are consistent with the DSMC results. This consistency is not surprising because the Fokker-Planck equation is actually an approximation of the Boltzmann equation [22]. Comparing with the DSMC method, the FPM method replaces the inter-particle collision with a continuum stochastic process. In this context, the FPM method can use much larger cell sizes and thus is more efficient for gas flows with small or moderate Knudsen (Kn) numbers. Considering the advantages of FPM method, Gorji et al. have also proposed a hybrid scheme with the DSMC method [23] for multi-scale gas flows and a variance reduction algorithm for low Mach number flows [24].

In the FPM method, the simulated molecules are tracked following the Langevin