Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2023-0068

Vol. **34**, No. 1, pp. 173-207
July 2023

General Synthetic Iterative Scheme for Unsteady Rarefied Gas Flows

Jianan Zeng[1], Wei Su[2,3] and Lei Wu[1,4,*]

[1] *Department of Mechanics and Aerospace Engineering, Southern University of Science and Technology, Shenzhen 518055, China.*
[2] *Division of Emerging Interdisciplinary Areas, The Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China.*
[3] *Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China.*
[4] *Guangdong-Hong Kong-Macao Joint Laboratory for Data-Driven Fluid Mechanics and Engineering Applications, Southern University of Science and Technology, Shenzhen 518055, China.*

Received 6 March 2023; Accepted (in revised version) 19 May 2023

Abstract. In rarefied gas flows, the spatial grid size could vary by several orders of magnitude in a single flow configuration (e.g., inside the Knudsen layer it is at the order of mean free path of gas molecules, while in the bulk region it is at a much larger hydrodynamic scale). Therefore, efficient implicit numerical method is urgently needed for time-dependent problems. However, the integro-differential nature of gas kinetic equations poses a grand challenge, as the gain part of the collision operator is non-invertible. Hence an iterative solver is required in each time step, which usually takes a lot of iterations in the (near) continuum flow regime where the Knudsen number is small; worse still, the solution does not asymptotically preserve the fluid dynamic limit when the spatial cell size is not refined enough. Based on the general synthetic iteration scheme for steady-state solution of the Boltzmann equation, we propose two numerical schemes to push the multiscale simulation of unsteady rarefied gas flows to a new boundary, that is, the numerical solution not only converges within dozens of iterations in each time step, but also asymptotically preserves the Navier-Stokes-Fourier limit in the continuum flow regime, when the spatial grid is coarse, and the time step is large (e.g., in simulating the extreme slow decay of two-dimensional Taylor vortex, the time step is even at the order of vortex decay time). The properties of fast convergence and asymptotic preserving of the proposed schemes are not only rigorously proven by the Fourier stability analysis for simplified gas kinetic models, but also demonstrated by several numerical examples for the gas kinetic models and the Boltzmann equation.

*Corresponding author. *Email addresses:* wul@sustech.edu.cn (L. Wu), 12031255@mail.sustech.edu.cn (J. Zeng), weisu@ust.hk (W. Su)

AMS subject classifications: 76P05

Key words: Unsteady rarefied gas flow, general synthetic iterative scheme, fast convergence, asymptotic Navier-Stokes preserving.

1 Introduction

Rarefied gas flows have attracted significant research interests in the past decades due to their wide range of engineering applications, including space vehicle re-entry, microelectromechanical system processing, and shale gas extraction. These flows are characterized by the Knudsen number Kn, which is defined as the ratio of mean free path λ (or mean collision time t_c) of gas molecules to the characteristic flow length L (or time/period t_0). Only when the Knudsen number is small can the rarefied gas dynamics be well described by macroscopic equations in the bulk flow region [1], such as the Euler, Navier-Stokes-Fourier (NSF), Burnett, super-Burnett [2], and (regularized) Grad 13 and 26 moments equations [3]; see the short review on the performance of dozens macroscopic equations [4]. Also noted that although the lattice Boltzmann method can simulate the Poiseuille flow with the tuning of effective viscosity [5,6], they cannot be applied to general rarefied gas flows [7]. For general values of Knudsen number, however, the Boltzmann equation or simplified gas kinetic equations, which uses the velocity distribution function to describe the gas dynamics at the mesoscopic level, should be used.

Since the velocity distribution function is defined in the six-dimensional phase space, the computational cost of memory and time for solving gas kinetic equations is huge. Thus, many numerical methods are proposed to solve the kinetic equations under a numerical scale larger than the kinetic one [8–15], that is, the spatial grid size $\Delta x \gg \lambda$, and/or the time step $\Delta t \gg \tau_c$. Some schemes asymptotically preserve the Euler limit, as they become a consistent discretization of the Euler equations when $\mathrm{Kn} \to 0$ [9,10]. Nevertheless, from a practical point of view, the Euler equations cannot be applied to most flows, even when the Knudsen number is small. For instances, in the Poiseuille flow [16] and Rayleigh-Brillouin scattering [17], the flow velocity and density perturbation scale as $1/\mathrm{Kn}$. If the Euler equations are used, they become divergent, which is not physical. Therefore, some numerical schemes are designed to asymptotically preserve the NSF limit when $\Delta t \gg \tau_c$ [11,12], under the assumption that the spatial derivatives are handled exactly. Recently, it is found that the NSF limit can be captured by the (discrete) unified gas-kinetic scheme, when both the time step and spatial cell size are much larger than the corresponding kinetic scales [13,14,18,19]: $\Delta x \sim \sqrt{\mathrm{Kn}} L \gg \lambda$ and $\Delta t \sim \sqrt{\mathrm{Kn}} t_0 \gg \tau_c$.

In reality, rarefied gas flows are intrinsically multiscale, say, in the two-dimensional thermal edge flow in the (near) continuum flow regime where the Knudsen number is small [17], the spatial grid size varies by several orders of magnitude: inside the Knudsen layer (which occupies a spatial region within a few mean free path away from the solid walls) $\Delta x \sim \lambda \sim 0.001$, while in the bulk region it is at a much larger hydrodynamic scale: