Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2021-0026

Vol. **31**, No. 3, pp. 816-868
March 2022

Kinetic Slip Boundary Condition for Isothermal Rarefied Gas Flows through Static Non-Planar Geometries Based on the Regularized Lattice-Boltzmann Method

Jean-Michel Tucny[1], David Vidal[1], Sébastien Leclaire[1] and François Bertrand[2,*]

[1] *Mechanical Engineering Department, Polytechnique Montral, P.O. Box 6079, Stn. CV, Montréal, QC, CANADA, H3C 3A7.*
[2] *Chemical Engineering Department, Polytechnique Montral, P.O. Box 6079, Stn. CV, Montréal, QC, CANADA, H3C 3A7.*

Communicated by Kun Xu

Received 4 February 2021; Accepted (in revised version) 2 November 2021

Abstract. The simulation of rarefied gas flows through complex porous media is challenging due to the tortuous flow pathways inherent to such structures. The Lattice Boltzmann method (LBM) has been identified as a promising avenue to solve flows through complex geometries due to the simplicity of its scheme and its high parallel computational efficiency. It has been proposed to model the stress-strain relationship with the extended Navier-Stokes equations rather than attempting to directly solve the Boltzmann equation. However, a regularization technique is required to filter out non-resolved higher-order components with a low-order velocity scheme. Although slip boundary conditions (BCs) have been proposed for the non-regularized multiple relaxation time LBM (MRT-LBM) for planar geometries, previous slip BCs have never been verified extensively with the regularization technique. In this work, following an extensive literature review on the imposition of slip BCs for rarefied flows with the LBM, it is proven that earlier values for kinetic parameters developed to impose slip BCs are inaccurate for the regularized MRT-LBM and differ between the D2Q9 and D3Q15 schemes. The error was eliminated for planar flows and good agreement between analytical solutions for arrays of cylinders and spheres was found with a wide range of Knudsen numbers.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07

Key words: Lattice Boltzmann method (LBM), boundary condition (BC), rarefied flow, non-planar geometry.

*Corresponding author. *Email addresses:* `jean-michel.tucny@polymtl.ca` (J.-M. Tucny), `david.vidal@polymtl.ca` (D. Vidal), `sebastien.leclaire@polymtl.ca` (S. Leclaire), `francois.bertrand@polymtl.ca` (F. Bertrand)

1 Introduction

Porous media are among the most complex geometries found in nature and industry. The macroscopic transport properties of porous media, such as permeability, are determined by their microscopic structure. Detailed knowledge of flow fields inside porous media can thus provide a better understanding of this structure, allowing the systems or processes involving porous media to be optimized. Numerical simulations have attracted interest for their potential to determine porous media transport properties. Despite the increase in computational power in recent years, traditional CFD methods are still limited with respect to the direct simulation of gas flows through realistic three-dimensional porous media for two reasons: (1) the presence of multiple scales of characteristic length in the same porous medium, and (2) the solid-fluid boundaries with convoluted topologies often found inside porous media [1].

The presence of several magnitudes of characteristic length implies that regions where the molecular mean free path λ is comparable to the characteristic length of the flow L_C can occur throughout the domain. The Knudsen number $Kn=\lambda/L_C$ gives a measure of flow rarefaction by indicating the extent to which gas molecules propagate before collisions exchange momentum and energy between gas molecules. In the Knudsen layer, a 2λ region near solid surfaces, local thermodynamic equilibrium is not reached, the continuum hypothesis no longer applies, and the Navier-Stokes equations (NSEs) no longer represent gas flow dynamics. Four regimes of rarefaction can be considered based on Devienne's original classification: (1) continuous flow ($Kn<0.001$), (2) slip flow ($0.001<Kn<0.1$), (3) transition (or Knudsen) flow ($0.1<Kn<10$), and (4) free molecular flow ($Kn>10$) [2]. In the continuous flow regime, the NSEs can be used with no-slip boundary conditions (BCs). In the slip flow regime, gas molecules incoming from a region with a finite flow velocity contribute to a non-zero slip velocity at the boundary. However, the NSEs are still considered to be valid in the bulk of the flow. In the transition or Knudsen flow regime, the Knudsen layer becomes large compared to the bulk of the flow, and the NSEs become invalid. In the free molecular flow regime, collisions between gas molecules are negligible. Limits between those regimes may vary depending on the authors [3–9] and should depend on the physics involved [6–8] and the geometry. [9] Although the Boltzmann equation is generally accepted as valid for all Knudsen numbers, analytical solutions have been developed only for a few simple geometries [10–12].

The Lattice Boltzmann method (LBM) is an alternative and well-proven approach for solving gas flows through porous media [13–16]. It is based on a discretization of the Boltzmann equation in which populations with a finite velocity set evolve according to a propagation-collision scheme on a regular Cartesian grid with a finite-difference scheme in time. The local and explicit nature of the LBM enables its massive parallelization and thus the simulation of multiple scales of characteristic length in porous media. The representation of solid and fluid lattices with a simple Boolean geometry facilitates BC discretization. Given all these advantages, studies have been conducted using the LBM on gas flows through porous media in various research fields such as shale gas [17–54],