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Shift-periodic boundary condition for heat transfer computations in lattice Boltzmann method☆

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ABSTRACT

With the developments in computational techniques, detailed simulations of flow thermomechanics and other phenomena in complex geometries, such as granular or porous media, are attracting increasing interest. Recently, the lattice Boltzmann method (LBM) is more and more often applied for such computations. In this work, we present a novel numerical scheme of shift-periodic boundary conditions for the internal energy distribution function in thermal LBM. As validation cases, we consider flow past an array of heated obstacles in regular and random arrangements, akin to the granular media geometry. The quality of the proposed shift-periodic scheme is documented and the LBM results are presented for temperature profiles. The developments proposed here are also of interest for volume-averaged modeling of porous media heat transfer.

1. Introduction

Recently, there is a growing interest in detailed or multiscale simulations of geometrically-complex flow systems, including the account of coupled phenomena. The analysis at different scales has become possible thanks to advances in computer power and developments of new computational methods. Physically-complex porous media flows with heat transfer and possibly with chemical reactions make a particular example of such flows. They are present in a number of technological processes (the power generation systems) and devices (the chemical and process engineering applications). In numerical computations, the porous medium is often dealt with as a representative element of volume (REV) to simulate various phenomena at the level of a single pore. The physico-chemical and geometrical complexities imply that more traditional methods of computational fluid dynamics (CFD) reveal to be expensive as far as detailed modeling is concerned. Therefore, our longer-term idea is to develop a multiscale approach with microscopic, or single-pore level, 3D/2D computations in the REV domain, followed by a macroscopic, physically-sound analysis of the process in terms of an averaged (1D/2D), unsteady model. In general, multiscale modeling offers fascinating perspectives in fluid dynamics; however, it is a demanding approach in terms of model developments. One needs to provide a detailed description of geometry (at the REV level and also at level below) and numerical tools, including relevant schemes of physically sound inlet/outlet boundary conditions.

One of the numerical tools (operating at the meso-scale level) that has recently gained considerable attention of the scientific and industrial communities is the lattice Boltzmann method (LBM). The method has proven suitable for simulation of viscous and nearly incompressible flows as well as convective heat transfer in simple and complex geometries; see [1] for a comprehensive introduction. The LBM has already attracted interest as an alternative tool of computational fluid dynamics, more and more used for modeling fluid–structure interactions [2, 3], chemical reactions and species transport, non-Newtonian flows [4], turbulence [5, 6], etc. Coupled LBM approaches are also reported; in [7] authors couple LB with discrete ordinates method for solving conduction and radiation heat transport problem. Li et al. in [8] couple LB with finite-volume method for modeling of the convective melting process.

As a first development step towards the physically-sound description of the coking process, the authors applied the LBM to simulate fluid flow past a cylinder and in simple granular (or porous) media [9]. In the second step, we have dealt with non-isothermal flows in a simple and complex geometry [10]. The present work addresses the problem of formulation and implementation of shift-periodic thermal conditions at the inlet and outlet boundaries of the REV domain (the bed of grains, like the coal grains during the coking process). In the case of fluid flow, the LBM formulation of

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shift-periodic condition for velocity in pressure-driven flow was first proposed and verified by Zhang and Kwok [11]. Their original proposal was subject to subsequent modifications; for example, Kim and Pitsch [12] have proposed a higher-accuracy, generalized formula applicable for fluid flows without constraints on velocity, otherwise typical of LBM applications. A few years later, Gräser and Grimm [13] proposed an extended scheme, accounting for adaptivity. This formulation guarantees that the scheme can also be used for complex cases where geometry of the single unit cell is not symmetric. There, the pressure gradient perpendicular to the main flow direction (occurring, e.g., through a lack of symmetry, also with respect to the momentum), is adjusted by a controller loop. Regarding heat transfer simulations in LBM, to the best knowledge of the authors, a scheme for periodic condition with a temperature difference between the inlet and the outlet is proposed here for the first time.

The shift-periodic condition is understood here as a practical concept for periodic geometries where the difference of a relevant variable (such as the pressure or temperature) between inlet and outlet drives the flow or results from heat transfer. In case of fluid flow, the pressure gradient is usually applied, whereas for heat transfer it is sometimes desirable to introduce the inlet/outlet temperature difference. Generally, the possibility to use the proposed scheme and shift-periodic boundary condition is of practical interest. In case of fluid flow, a number of results are known from the literature where the pressure drop in a given geometry can be calculated from empirical correlations. A well-known example is the Darcy law with permeability determined by, e.g., the Carman–Kozeny correlation. As far as heat transfer is concerned, some situations where the shift-periodic boundary condition is needed are presented in Fig. 1. The fluid flow is driven by the imposed pressure drop. As the first case, we consider distributed heat sources in the domain, in the form of the hot/cold obstacles (plot a). Alternatively, a non-zero heat flux at the side boundaries may be considered (plot b). In description of these cases, one has to consider an overall temperature difference between inlet and outlet. We treat obstacles in the domain as heat sources (see Fig. 1a) and, for the sake of simplicity, we assume periodic boundary conditions in the cross-stream direction. Such a configuration with a regular arrangement of obstacles was used as the validation test case by Kuwahara et al. [14]. There, obstacles were treated as heat sources with the same temperature, different than that of the inlet flow. We address this case in detail in Sec. 3.1. This geometry was next used by other authors (see [10, 15]) for comparison and validation purposes; also correlations for the Nusselt number were proposed there.

2. Numerical modeling

2.1. Lattice Boltzmann method

In the present work we use the lattice Boltzmann method, with the fluid density and velocity solved in terms of the density distribution function (denoted by f) as presented in [16]. In addition, the temperature field is found from the internal energy density distribution function (IEDDF, denoted by g), see [17–19]. The form of all LB equations used here is similar; for advection of both f and g, we use the discretization schemes D2Q9 for 2D and D3Q19 for 3D; symbolically, $f(\mathbf{x}, t, \mathbf{e}) \to f_i(\mathbf{x}, t)$. The resulting evolution equations (with the BGK simplification, see [1]) are

$$f_i(\mathbf{x} + \mathbf{e}_i\delta t, t + \delta t) = f_i(\mathbf{x}, t) + \delta t(f_i^{eq} - f_i)\tau_\nu^{-1} \quad (1)$$

$$g_i(\mathbf{x} + \mathbf{e}_i\delta t, t + \delta t) = g_i(\mathbf{x}, t) + \delta t(g_i^{eq} - g_i)\tau_\alpha^{-1}$$

where $\mathbf{e}_i$ are discrete velocity directions for advection of the distribution functions on the lattice. Here, f_i^{eq} and g_i^{eq} are the equilibrium distributions:

$$f_i^{eq} = \rho\Omega_i\left[1 + \frac{3}{c^2}\mathbf{e}_i\cdot\mathbf{u} + \frac{4.5}{c^4}(\mathbf{e}_i\cdot\mathbf{u})^2 - \frac{1.5}{c^2}u^2\right]$$

$$g_i^{eq} = \theta\Omega_i\rho\left[a_t + b_t\mathbf{e}_i\cdot\mathbf{u} + c_t(\mathbf{e}_i\cdot\mathbf{u})^2 + d_t u^2\right] \quad (2)$$

where the IEDDF coefficients a_t, b_t, c_t, d_t are not constant and depend on the discretization model and the advection direction i (see [18]). Ω_i are the weight coefficients; θ and ρ are the temperature and density, respectively, at a given node. The relaxation parameters τ_ν and τ_α for f and g distributions, respectively, are functions of crucial physical properties: viscosity ν and heat transfer coefficients α (of solid and fluid). The macroscopic flow density ρ, velocity $\mathbf{u}$ and temperature θ at each lattice node are found from suitable averaging [1]:

$$\rho = \sum_i f_i, \qquad \mathbf{u} = \rho^{-1}\sum_i \mathbf{e}_i f_i, \qquad \theta = \rho^{-1}\sum_i g_i.$$

2.2. Boundary schemes

At the solid/fluid interface, we use the boundary conditions for fluid flow and heat transfer translated in the LBM variables. They are the no-slip condition for velocity and a known temperature assumed at the surface of heated obstacles (see Fig. 1a). Alternatively, the temperature field of obstacles can also be modeled by LBM (details are given in Sec. 3). For modeling purposes we use the standard bounce-back scheme for flow velocity at the solid–fluid interface [1]; for heat transfer we use the boundary scheme presented by He et al. [17].

At the side boundaries of computational domain, parallel to the flow direction, we use the standard periodic condition. In the scheme, all distribution functions with the advection vector pointing outside (leaving the domain) are copied to the opposite boundary. At the cross-stream boundaries, perpendicular to the main flow direction, we use the shift-periodic boundary conditions for f (where the pressure drop between inlet and outlet is calculated from the Darcy

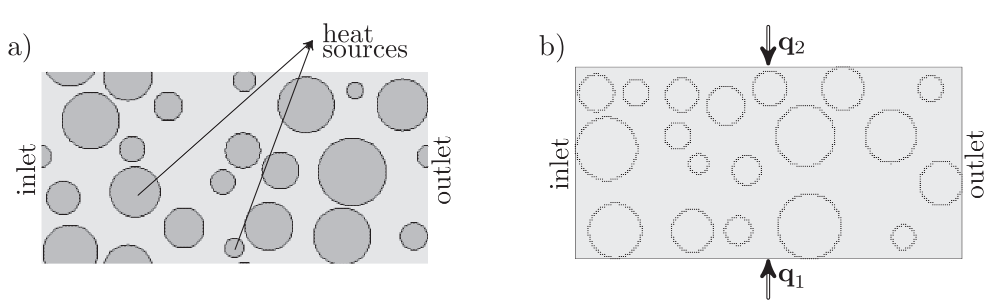

Fig. 1. Examples of simulation cases where shift-periodic type boundary condition is needed.