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A Generalized Local Grid Refinement Approach for Modeling of Multi-Physicochemical Transports by Lattice Boltzmann Method

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Abstract. The multi-physical transport phenomena through the different size geometries are studied by developing a general local grid refinement approach for lattice Boltzmann methods. Revisiting the method of local fine patches on the coarse grid, through the Chapman-Enskog expansion, the multi-physicochemical source terms such as ion electro-migration, heat source, electric body force, and free net electric charge density can be rigorously incorporated to the rescaling relations of the distribution functions, which interchange between fine and coarse grids. We propose two general local refinement approaches for lattice Boltzmann for momentum and advection-diffusion equations with source terms. To evaluate our algorithm, (i) a body-force driven Poiseuille flow in a channel; (ii) an electro-osmotic flow in which the coupled Poisson-Nernst-Planck with Navier-Stokes equations for overlapped and non-overlapped electric double layers; (iii) a symmetric and asymmetric 1D and 2D heat conduction with heat generation in a flat plate; and (iv) an electric potential distribution near a charged surface, are modeled numerically. Good agreements with the available analytical solutions demonstrated the robustness of the proposed algorithm for diffusion or advection-diffusion equations, which may be coupled or decoupled. The present model may broaden the applications of local grid refinement for modeling complex transport phenomena, such as multi-physicochemical transport phenomena in different size geometries.

AMS subject classifications: 65N50, 74S30

Key words: Local grid refinement, lattice Boltzmann model, source term, multiscale geometry, multi-physics.

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1 Introduction

At recent decade, investigating mechanisms of multi-physicochemical transport phenomena has been of great interests with important applications in micro- and nanosystems [1–7]. To study the transport mechanism, the uniform grid lattice Boltzmann method as an efficient and inexpensive method has been widely used recently [8–12]. However, in real applications, for different size (e.g., micro-nano conjunction) problems or problems with a high gradient of physical properties region, the uniform grids would not retain the major superiority of the lattice Boltzmann method over other computational methods. To deal with this challenge, several attempts have been drawn to improve the adequate grid resolution of the lattice Boltzmann method [13–19]. For this purpose, the local grid refinement method has been proposed based on the concept of the hierarchical grid refinement with higher applicability, accuracy, and efficiency [20].

The first employing of second-order local grid refinement technique for the lattice Boltzmann model was developed by Filippova and Hanel [21], which hereinafter is so called as FH model. In their work, the whole domain is covered by a coarse grid. For regions where large changes of macroscopic properties are expected, fine grids are superposed to the coarse grid. In addition, for the adaptive mesh refinement methods, one can adapt the size and number of superposed fine patches [22]. By considering the same viscosity and, as a result, the same Reynolds number for two grids, the relaxation parameters could be redefined for fine grids. For a pressure driven flow over a circular cylinder, the drag (C_D), lift (C_L) and pressure difference (ΔP) coefficients have good agreements with the available experiments [23]. Later, Filippova and Hanel [20] developed their model in which the molecular velocities in the fine and coarse grids could be different. It should be mentioned that the Reynolds number for both fine and coarse grids is retained identical. Lin and Lai [24] proposed a simpler algorithm without considering the rescaling of distribution functions when transformed from coarse to fine grid and vice versa. However, this assumption may impose some inaccuracy since the non-equilibrium part of the distribution function has been ignored. Dupuis and Chopard [25] showed that how the approximation of the non-equilibrium distribution function without external force could resolve the singularity problem of the FH model when the relaxation parameters were close to 1.0. For the applicability of the local grid refinement technique, Rohde et al. [26] indicated that their methods were capable of accurately describing the experimental data. To extend the applicability of modeling different flow regimes, Lagrava et al. [27] proposed a method to interchange data for fine-coarse grids under high Reynolds number. Moreover, Eitel-Amor et al. [28] proposed a local hierarchical adaptive grid refinement using the cell-centered lattice structure. They demonstrated that the proposed method could be applied for modeling high Reynolds number flow regimes over a sphere or a circular cylinder. Considering other transport phenomena, Liu et al. [29] reported a two-dimensional multi-block lattice Boltzmann model for solute transport in a shallow water based on the advection-diffusion equation without source term. Stiebler et al. [30] extended the advection-diffusion LB scheme for the hierarchical grids based on