Optimization of the Multiple-Relaxation-Time Micro-Flow Lattice Boltzmann Method

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Abstract: Evaluation and optimization of the multiple-relaxation-time (MRT) lattice Boltzmann method for micro-flows (μ -flow LBM) are performed with the two-dimensional nine discrete velocity (D2Q9) model. The MRT μ -flow LBM consisting of the combination of bounce-back and full diffusive (CBBFD) wall boundary condition is considered. Based on the discussion of Chai et al. (2010), the presently applied CBBFD model and relaxation time for heat flux τ_a satisfy the second-order slip boundary condition. However, modification to the MRT model of Chai et al. (MRT-C) is made to the relaxation time for the moments related to the stress τ_s by introducing the psi function (Stops, 1970; Guo et al., 2006). This modified MRT-C model (MRT-Cm1) and further modified model (MRT-Cm2) by changing the coefficients of the second-order slip velocity to the coefficients of Mitsuya (1993) are evaluated. As shown in Fig.1, since the MRT-Cm2 model performs best among the evaluated models including the one by Verhaeghe et al. (MRT-V) in predicting slip velocities and flow rates of Poiseuille flows in the range of Knudsen number 0.01<Kn<10, it is further evaluated in the flow around an obstacle situated in a nanochannel. Two kinds of obstacles are considered: a square cylinder (Suga et al., 2010) and a triangular prism. For producing the reference data of the triangular prism flow, the classical molecular dynamics simulation using Lennard-Jones potential is also performed in the present study. An interpolation scheme is applied to the CBBBFD wall boundary model for describing the surfaces of the triangular prism. As shown in Figs.2 and 3, it is confirmed that the MRT-Cm2 model performs much better than the SRT μ -flow LBM of Niu et al. (2007) (SRT-N).

Keywords: lattice Boltzmann method, Knudsen number, molecular dynamics simulation, Poiseuille flow, obstacle flow.

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Figure 1: Dependency of the flow characteristics on Kn; (a) velocity scaling at wall and centerline of the channels, and (b) flow rate.

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Figure 2: Flow around a square cylinder in a nanochannel at Kn=0.11; (a) schematic view, (b) streamwise velocity at x/H = 0.0, (c) streamwise velocity at x/H = 0.5, (d) wall-normal velocity at x/H = 0.25.



Figure 3: Flow around a triangular prism in a nanochannel at Kn=0.15; (a) schematic view, (b) streamwise velocity at x/H = 0.0, (d) streamwise velocity at x/H = 0.5, (c) wall-normal velocity at x/H = 0.43.

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