Finite-difference lattice Boltzmann methods for binary miscible fluids

Aiguo Xu

Department of Physics, Yoshida-South Campus, Kyoto University, Sakyo-ku, Kyoto, 606-8501, Japan

In recent years, the lattice Boltzmann method (LBM) has attracted considerable attention and has been regarded as a promising alternative numerical scheme for simulating fluid flows[1]. The basic reasons are (i) that the Euler and the Navier-Stokes equations have their basis in the Boltzmann equation – the former can be derived from the latter under the hydrodynamic limit by using the Chapmann-Enskog analysis, which makes possible to understand the macroscopic properties of fluids from the microscopic level, and (ii) that analytical solutions of the Boltzmann equation are available only in very limited cases. The standard lattice Boltzmann method (SLBM) was developed from the lattice gas cellular automata (LGCA) and later it was directly derived from the Boltzmann equation. Since work partly as a floating-number counterpart of the Boolean LGCA, within the SLBM one evolution step is split as a propagation and a collision ones. This treatment is also referred to as a special form of the finite-difference scheme. For methods developed along this line, it should be noted that one of the main ideas driving the initial LGCA was to produce the simplest microdynamics that yields hydrodynamic behavior. A second way to formulate a discrete Boltzmann equation is referred to as the finite-difference lattice Boltzmann method (FDLBM). Within this method the general finite-difference schemes are used. Within this scheme the physical symmetry of hydrodynamic systems can be more conveniently recovered by the used discrete velocity model (DVM). The SLBM and the FDLBM stand for two different numerical schemes to discretize the Boltzmann equation. The two kinds of schemes are expected to be complementary in the LBM studies.

Various merits are expected from an appropriately designed LBM: (i) simple schemes, (ii) linear advective terms, (iii) high resolution for shock wave computation, (iv) interparticle interactions can be easily incorporated if needed, etc. Additionally, in systems involving interfaces, the interfaces separating different components/domains are difficult for the conventional Navier-Stokes solver to track due to the complex geometry and possible phase change. In such cases, the LBM is expected to be a convenient tool. In recent years some LBMs for multicomponent systems have been attempted and developed. In the poster presentation we will show three new FDLBMs for binary mixtures. To understand the necessity and merits of the new FDLBMs, we first briefly summarize the present research status of the LBMs for multicomponent fluids: (i) Most existing methods belong to the SLBM; (ii) Most existing methods are based on the single-fluid theory; (iii) In Ref. [2] a SLBM based on a two-fluid kinetic theory was proposed and developed. It is a pity that within this method the mass conservation does not hold for each individual species at the Navier-Stokes level; (iv) Nearly all the studies are focused on isothermal and nearly incompressible systems. Therefore, designing LBMs for binary mixtures based on two-fluid kinetic theory is still an open project. We expect that the formulated FDLBMs will partly fill this gap.

In the poster presentation, the based kinetic theory will be briefly reviewed and the corresponding hydrodynamic equations will be given. Then three FDLBMs will be formulated and numerically verified. They are for, respectively, (i) the isothermal Navier-Stokes equations, (ii) the thermal and compressible Euler equations, (iii) the complete Navier-Stokes equations.

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^[1] S. Succi, The Lattice Boltzmann Equation (Oxford University Press, New York, 2001).

^[2] L.S. Luo and S. S. Girimaji, Phys. Rev. E 66, 35301(R) (2002); *ibid.* 67, 36302 (2003).