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TWO COMPONENT LATTICE BOLTZMANN MODEL WITH FLUX LIMITER TECHNIQUES

Artur CRISTEA, Victor SOFONEA

Laboratory for Numerical Simulation and Parallel Computing in Fluid Mechanics
Center for Fundamental and Advanced Technical Research, Romanian Academy
Bd. Mihai Viteazul 24, R-1900, Timişoara, Romania
e-mails: f1astra@acad-tim.utt.ro; sofonea@acad-tim.utt.ro

Flux limiters techniques are used in a finite difference lattice Boltzmann model for two component fluid systems. The Lattice Boltzmann model was successfully applied to investigate the phase separation process, as well as the behaviour of the magnetic fluid – nonmagnetic fluid interface subjected to the action of an external magnetic field.

1. INTRODUCTION

Lattice Boltzmann (LB) models [1,2,3,4,5] provide an alternative to current methods of computational fluid dynamics. Unlike standard numerical techniques based on the discretization of the macroscopic fluid equations, LB models are based on the physics at the mesoscopic scale, while the macroscopic level phenomena are recovered from evolution equations. For a two component fluid system, we have two sets of distribution functions $\{f_i^\sigma(\mathbf{x},t),\ i=0,1,\ldots \mathrm{N}\}(\sigma=0,1)$. The distribution function $f_i^\sigma(\mathbf{x},t)$ expresses the probability to find in node $\mathbf{x}$ of the lattice a particle of species σ having the velocity $\mathbf{e}_i^\sigma$. The evolution equations for the distribution functions are derived from the Boltzmann equation after discretisation of the phase space [6]:

$$\partial_t f_i^\sigma(\mathbf{x},t)+\mathbf{e}_i^\sigma\cdot\nabla f_i^\sigma(\mathbf{x},t)=-\frac{1}{\tau}[f_i^\sigma(\mathbf{x},t)-f_i^{\sigma,eq}(\mathbf{x},t)]+\frac{1}{k_BT}\mathbf{F}^\sigma(\mathbf{x},t)\cdot[\mathbf{e}_i^\sigma-\mathbf{u}(\mathbf{x},t)]f_i^{\sigma,eq}(\mathbf{x},t)$$
$$\sigma=0,1;\qquad i=0,1,\ldots \mathrm{N} \tag{1}$$

Here τ are relaxation times and $\mathbf{F}^\sigma(\mathbf{x},t)$ is the force acting on a particle of species σ in lattice node $\mathbf{x}$ at time t. In the two dimensional (2D) case, N=8 and:

$$\mathbf{e}_i^\sigma=\begin{cases}(0,0) & ,\quad i=0\\ c^\sigma\left(\cos\frac{(\mathrm{i}-1)\pi}{2},\sin\frac{(i-1)\pi}{2}\right) & ,\quad i=1,\ldots 4\\ c^\sigma\sqrt{2}\left(\cos\frac{(2\mathrm{i}-9)\pi}{4},\sin\frac{(2i-9)\pi}{4}\right) & ,\quad i=5,\ldots 8\end{cases} \tag{2}$$

where $c^\sigma=\sqrt{k_BT/\chi m^\sigma}$ is the thermal speed of particles belonging to component σ (k_B is the Boltzmann constant, T is the temperature of the system, m^σ is the mass of particles of species σ and $\chi=1/3$).
The equilibrium distribution functions:

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$$f_i^{\sigma,eq} = w_i n^\sigma \left[1 + \frac{\mathbf{e}_i^\sigma \cdot \mathbf{u}}{\chi (c^\sigma)^2} + \frac{(\mathbf{e}_i^\sigma \cdot \mathbf{u})^2}{2\chi^2 (c^\sigma)^4} - \frac{\mathbf{u}\cdot\mathbf{u}}{2\chi (c^\sigma)^2} \right] \tag{3}$$

are expressed as a series expansion in the barycentric velocity [7]:

$$\mathbf{u} = \mathbf{u}(\mathbf{x},t) = \frac{m^0 n^0 \mathbf{u}^0 + m^1 n^1 \mathbf{u}^1}{m^0 n^0 + m^1 n^1} \tag{4}$$

where $n^\sigma = \sum_{i=0}^{N} f_i^\sigma(\mathbf{x},t)$ is the local particle number density of component σ. The weight factors in (3) are: $w_0 = 4/9,\ \ w_1 = \ldots w_4 = 1/9,\ \ w_5 = \ldots = w_8 = 1/36$.

2. FLUX LIMITER TECHNIQUES

The phase space discretized Boltzmann equations (1) may be solved numerically by using an appropriate finite difference scheme defined on the lattice. When using a characteristic based finite difference scheme (Figure 1 shows the characteristic lines for two particular directions), the forward Euler finite difference is used to compute the time derivative and the distribution functions $f_{i,j}^\sigma$ are updated at each lattice node j, at time step n+1 in accordance with [8]:

$$f_{i,j}^{\sigma,n+1} - f_{i,j}^{\sigma,n} + \delta t \mathbf{e}_i^\sigma \cdot (\nabla f_i^{\sigma,n})_j = -\frac{\delta t}{\tau}[f_{i,j}^{\sigma,n} - f_{i,j}^{\sigma,eq,n}] + \frac{\delta t}{k_B T}\mathbf{F}_j^{\sigma,n} \cdot [\mathbf{e}_i^\sigma - \mathbf{u}_j^n] f_{i,j}^{\sigma,eq,n} \tag{5}$$

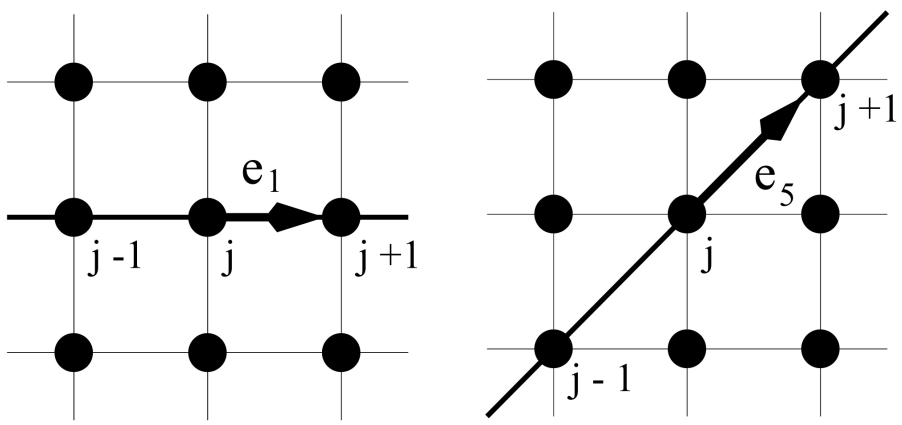

Figure 1 Characteristic lines for two particular lattice directions: i=1 (left) and i=5 (right)

Total Variation Diminishing (**TVD**) techniques and, in particular, flux limiter techniques [9,10] are currently used to improve the numerical stability of finite difference schemes. When using a flux limiter technique to compute space derivatives, the left hand side of (5) becomes:

$$f_{i,j}^{\sigma,n+1} - f_{i,j}^{\sigma,n} + \delta t \mathbf{e}_i^\sigma \cdot (\nabla f_i^{\sigma,n})_j = f_{i,j}^{\sigma,n+1} - f_{i,j}^{\sigma,n} + CFL^\sigma [F_{i,j+1/2}^{\sigma,n} - F_{i,j-1/2}^{\sigma,n}] \tag{6}$$

where $CFL^\sigma = c^\sigma \delta t / \delta x$ is the Courant-Friedrichs-Levy number of the component σ and

$$\begin{aligned} F_{i,j+1/2}^{\sigma,n} &= f_{i,j}^{\sigma,n} + \frac{1}{2}(1 - CFL^\sigma)\left[f_{i,j+1}^{\sigma,n} - f_{i,j}^{\sigma,n}\right]\psi(\theta_{i,j}^{\sigma,n}) \\ F_{i,j-1/2}^{\sigma,n} &= f_{i,j-1}^{\sigma,n} + \frac{1}{2}(1 - CFL^\sigma)\left[f_{i,j}^{\sigma,n} - f_{i,j-1}^{\sigma,n}\right]\psi(\theta_{i,j-1}^{\sigma,n}) \end{aligned} \tag{7}$$

are numerical fluxes. The flux limiter $\psi(\theta_{i,j}^{\sigma,n})$ is expressed as a function of the smoothness [9,10]:

$$\theta_{i,j}^{\sigma,n} = \frac{f_{i,j}^{\sigma,n} - f_{i,j-1}^{\sigma,n}}{f_{i,j+1}^{\sigma,n} - f_{i,j}^{\sigma,n}} \tag{8}$$

Standard finite difference schemes are recovered from (6) for two particular values of the flux limiters: $\psi(\theta_{i,j}^{\sigma,n}) = 0$ (upwind scheme) and $\psi(\theta_{i,j}^{\sigma,n}) = 1$ (Lax Wendroff scheme).

A wide choice of flux limiters is available in the literature [9,10]. In this paper, we will use the Monitorized Central Difference (MCD) flux limiter [9].

$$\psi(\theta_{i,j}^{\sigma,n}) = \begin{cases} 0 & , \quad \theta_{i,j}^{\sigma,n} \le 0 \\ 2\theta_{i,j}^{\sigma,n} & , \quad 0 \le \theta_{i,j}^{\sigma,n} < \frac{1}{3} \\ \dfrac{1+\theta_{i,j}^{\sigma,n}}{2} & , \quad \frac{1}{3} \le \theta_{i,j}^{\sigma,n} < 3 \\ 2 & , \quad \theta_{i,j}^{\sigma,n} > 3 \end{cases} \tag{6}$$

3. THE FORCE TERM

The total force acting on particles of species σ is a sum of three terms:

$$\mathbf{F}^{\sigma} = \mathbf{F}^{s,\sigma} + \mathbf{F}^{d,\sigma} + \mathbf{F}^{e,\sigma} \tag{9}$$

The first term:

$$\mathbf{F}^{s,\sigma} = \frac{\lambda}{\chi c^{\sigma} \delta x} \sum_{i=1}^{N} w_i n^{\bar{\sigma}} (\mathbf{x} + \mathbf{e}_i^{\bar{\sigma}} \delta x / c^{\bar{\sigma}}) \, \mathbf{e}_i^{\bar{\sigma}} \quad , \quad \bar{\sigma} = 1 - \sigma \tag{10}$$

where λ is the measure of the interparticle interaction, is responsible for the phase separation in the two component fluid system. The second force term

$$\mathbf{F}^{d,\sigma} = \begin{cases} 0 & , \quad \sigma = 0 \\ -n^1(\mathbf{x}) \displaystyle\sum_{i=1}^{N} G_i^d n^1(\mathbf{x} + \mathbf{e}_i^1 \delta x / c^1) \mathbf{e}_i^1 & , \quad \sigma = 1 \end{cases} \tag{11}$$

is responsible for the dipolar interaction. This term is characteristic to magnetic fluids where dipolar interaction is present between colloidal particles ($\sigma = 1$) dispersed in a carrier liquid ($\sigma = 0$). The dipolar interaction is controlled by the parameter $m = |\,\mathbf{m}\,|$ (the mean value of the magnetic moment carried by each particle), which enters the expression of the potential energy [11]:

$$G_i^d = \frac{w_i}{\chi c^1 \delta x} \left[\frac{m^2}{(\delta x)^2} - \frac{3(\mathbf{m} \cdot \mathbf{e}_i^1)^2}{(c^1 \delta x)^2} \right], \quad (i = 1 \ldots 8) \tag{12}$$

The third force term $\mathbf{F}^{e,\sigma}$, accounts for the action of external forces, e.g. gravity. In this paper we considered only the case $\mathbf{F}^{e,\sigma} = 0$.

4. PHASE SEPARATION

As discussed in [12], the value of the order parameter $\Delta n = n^0 - n^1$ in the equilibrium state is the solution of the equation:

$$\frac{1+\Delta n}{1-\Delta n} = \exp(\lambda \Delta n) \tag{13}$$

Phase separation ($\Delta n \neq 0$) occurs when the interaction parameter λ in the force term (10) exceeds the critical value $\lambda_{critical} = 2.0$ (Figure 2). However, the values of the order parameter Δn recovered during simulations are subjected to errors induced by the discretisation procedure of standard finite difference schemes [8,13] like the upwind scheme. As seen in Figure 2, the values of Δn become very close to the theoretical curve (13) when the MCD flux limiter is used instead of the standard upwind scheme. Figure 3 shows the spatial dependence of the order parameter Δn in a 2D fluid system with two components, for $\lambda = 3.5$, for both schemes. The presence of a transition region (interface) between the two phases is clearly observed. However, the absolute value $|\ \Delta n\ |$ of the order parameter is smaller for the upwind scheme since the numerical diffusion (which alters the simulation results) is larger in this case.

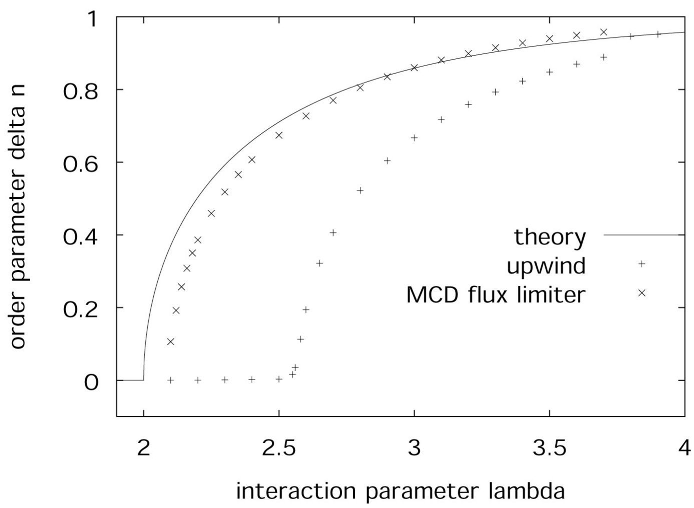

Figure 2 Dependence of the order parameter $\Delta n = n^0 - n^1$ vs. interaction parameter λ

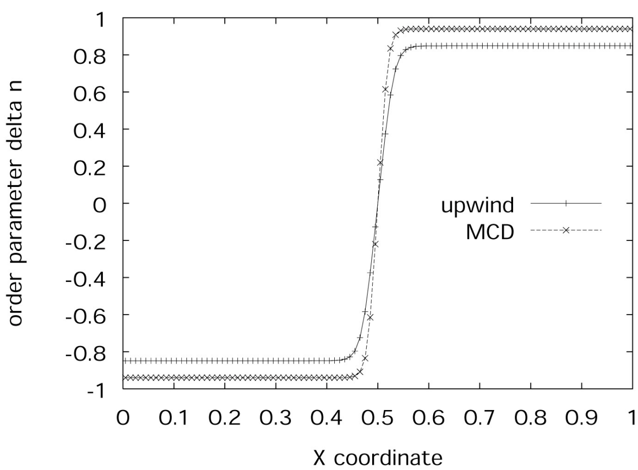

Figure 3 Spatial dependence of the order parameter $\Delta n = n^0 - n^1$ in two-phase system

5. MAGNETIC FLUID – NONMAGNETIC FLUID INTERFACE

The competition between dipolar interaction and surface tension forces, which are difficult to be investigated via computer simulations because of numerical instabilities generated by large density gradients in the interface region, gives rise to a rich variety of interface phenomena in magnetic fluids. We considered two cases to check the stability of our LB model with the MCD flux limiter. In the first case, a magnetic fluid drop was placed in a uniform magnetic field orientated along the horizontal direction. As expected [11,14], the drops elongates along the field direction when the magnetic field becomes larger (Figure 4a). In the second case, a gas bubble was placed in a magnetic fluid. Because of the reversed sign of the magnetic pressure [11], the elongation of the gas bubble is perpendicular to the horizontally applied magnetic field (Figure 4b).

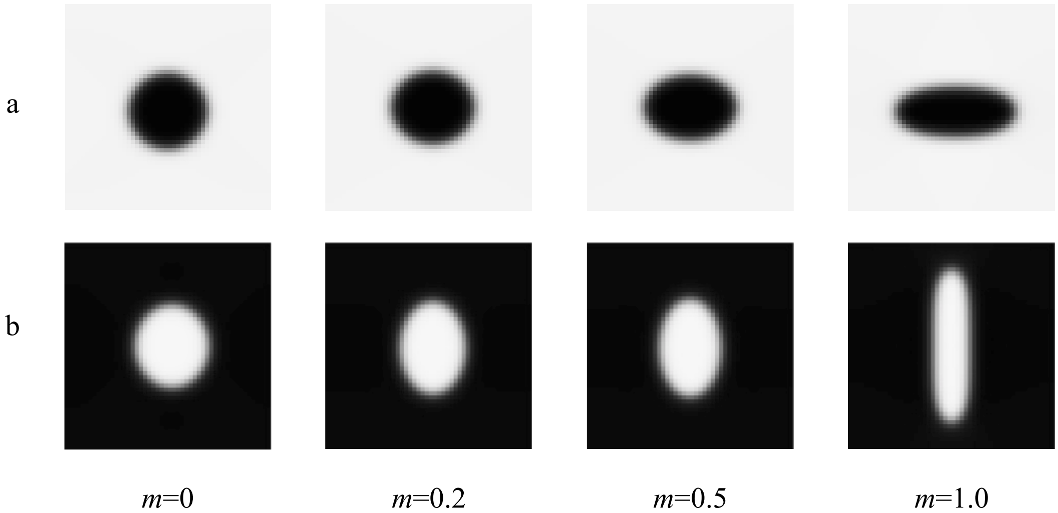

Figure 4. Deformation of a magnetic fluid drop (a) and of a gas bubble placed in magnetic liquid (b) for several values of the parameter *m*

6. CONCLUSIONS

In this paper we developed a flux limiter technique for lattice Boltzmann models. This technique provides a generalization of standard finite difference schemes and reduces substantially the numerical errors associated, e.g., to the upwind finite difference scheme, which are generated by the numerical diffusion. As a result, the phase diagram of the two component fluid system is closer to the theoretically derived curve when using the improved lattice Boltzmann model with flux limiter. The stability of this new model was checked in the case of a magnetic fluid – nonmagnetic fluid system, where large values of the density gradients, as well as of the dipolar interaction energy, are present in the interface region.

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Mechanics, Center for Fundamental and Advanced Technical Research, Romanian Academy, Timişoara). Parallel computing codes were developed using the Portable Extensible Toolkit for Scientific Computation (PETSc 2.1.3) developed at Argonne National Laboratory, Argonne, Illinois [17].

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