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FINITE DIFFERENCE LATTICE BOLTZMANN MODEL FOR LIQUID VAPOUR SYSTEMS

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A finite difference Lattice Boltzmann model for the Van der Waals liquid – vapour system is developed. Density and velocity profiles are derived using two different numerical schemes for the calculation of the force term in the Boltzmann evolution equation. Scalability of the parallel computing code on two computer clusters is also investigated.

1. INTRODUCTION

Lattice Boltzmann (LB) models [1,2,3,4,5] provide an alternative to current methods in computational fluid dynamics (CFD). Unlike conventional 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 which contain the force $\mathbf{F} = m\mathbf{a}$ acting on a fluid particle of mass *m.* Due to their local nature, LB models are suitable for parallel computing.

The starting point of LB models is the set of evolution equations for the distribution functions $f_i(\mathbf{x},t)$, which is recovered from the Boltzmann equation after discretisation of the phase space [6]:

$$\begin{aligned} &\partial_t f_i(\mathbf{x},t) + \mathbf{e}_i \cdot \nabla f_i(\mathbf{x},t) = \\ &-\frac{1}{\tau}[f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)] \\ &+\frac{1}{k_B T}\mathbf{F}\cdot[\mathbf{e}_i - \mathbf{u}(\mathbf{x},t)]f_i^{eq} \\ &i = 0,1,...N \end{aligned} \tag{1}$$

Here $\{\mathbf{e}_i\}$ is the discrete set of particle velocities, while position vectors $\mathbf{x}$ belong to a discrete lattice L. In the one dimensional (1D) case, N=2, and:

$$\mathbf{e}_i = \begin{cases} 0 & , \quad i = 0 \\ c & , \quad i = 1 \\ -c & , \quad i = 2 \end{cases} \tag{2}$$

where $c = \sqrt{\frac{k_B T}{\chi m}}$ is the thermal speed (k_B is the Boltzmann constant, T is the temperature of the system and $c = 1/3$).

The equilibrium distribution functions f_i^{eq} are expressed as a series expansion in the local velocity $\mathbf{u} = \mathbf{u}(\mathbf{x},t)$:.

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

The weight factors for the 1D case are: $w_0 = 2/3,\ w_1 = w_2 = 1/6$.

2. MACROSCOPIC EQUATIONS

The non-dimensional momentum conservation equation [6] of the 1D model is:

$$\partial_t(\rho\,\mathbf{u}) + \nabla(\rho\,\mathbf{uu}) = -\nabla p + \nu\nabla(\rho\,\nabla\mathbf{u}) + \rho\,\mathbf{a} \tag{4}$$

where ñ is the local fluid density and í is the fluid viscosity. To retrieve a non-ideal equation of state for the pressure $p = p(r,T)$, the force term should be:

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$$\mathbf{F} = m\mathbf{a} = -\frac{m}{\rho}\nabla(p_w - p_{id}) \tag{5}$$

where the Van der Waals pressure p_w [7] and respectively the ideal gas pressure p_{id} are:

$$\begin{aligned} p_w &= \frac{\rho T}{3-\rho} - \frac{3}{8}\rho^2 \\ p_{id} &= \chi c^2 \rho \end{aligned} \tag{6}$$

With these relations, taking into account the expression for the equilibrium distribution functions, the force term in the 1D LB equation becomes (up to second order in u):

$$\begin{aligned} &\frac{\mathbf{F}}{\chi c^2 m}[\mathbf{e}_i - \mathbf{u}] f_i^{eq} = \\ &-\frac{w_i}{m}\left[\frac{\mathbf{e}_i - \mathbf{u}}{\chi c^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})\mathbf{e}_i}{\chi^2 c^4}\right] \cdot \nabla(p_w - p_{id}) \end{aligned} \tag{7}$$

2. FINITE DIFFERENCE SCHEMES

The well-known Euler method and the upwind finite difference (FD) schemes [8] were used to compute the terms $\partial_t f_i$ and $\mathbf{e}_i \cdot \nabla f_i$ in Eq. (1), while two different FD schemes were considered for the pressure gradient in Eq. (7). The lattice spacing $dx = L/N$ is related to the length of the system L and the number of lattice nodes N. Using the notation $P(\mathbf{x},t) = p_w(\mathbf{x},t) - p_{id}(\mathbf{x},t)$, the CENTERED scheme reads:

$$\begin{aligned} &f_i(\mathbf{x}, t+\delta t) = f_i(\mathbf{x}, t) \\ &-\frac{c\delta t}{\delta x}[f_i(\mathbf{x}, t) - f_i(\mathbf{x} - \mathbf{e}_i\, \delta x/c, t)] - \\ &-\frac{w_i \delta t}{2m\delta x}\left[\frac{\mathbf{e}_i - \mathbf{u}(\mathbf{x}, t)}{\chi c^2} + \frac{\mathbf{e}_i\,(\mathbf{e}_i \cdot \mathbf{u}(\mathbf{x}, t))}{\chi^2 c^2}\right] \\ &\times[P(\mathbf{x} + \mathbf{e}_i\, \delta x/c, t) - P(\mathbf{x} - \mathbf{e}_i\, \delta x/c, t)] \\ &-\frac{\delta t}{\tau}\left[f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)\right] \end{aligned} \tag{8}$$

and the MIXED scheme reads:

$$\begin{aligned} &f_i(\mathbf{x}, t+\delta t) = f_i(\mathbf{x}, t) \\ &-\frac{c\delta t}{\delta x}\{[f_i(\mathbf{x}, t) - f_i(\mathbf{x} - \mathbf{e}_i\, \delta x/c, t)] \\ &+\frac{w_i}{m\chi c^2} \times [P(\mathbf{x}, t) - P(\mathbf{x} - \mathbf{e}_i \delta x/c, t)]\} \\ &-\frac{w_i \delta t}{2m\delta x}\left[-\frac{\mathbf{u}(\mathbf{x}, t)}{\chi c^2} + \frac{\mathbf{e}_i(\mathbf{e}_i \cdot \mathbf{u}(\mathbf{x}, t))}{\chi^2 c^4}\right] \\ &\times\left[P(\mathbf{x} + \mathbf{e}_i \delta x/c, t) - P(\mathbf{x} - \mathbf{e}_i \delta x/c, t)\right] \\ &-\frac{\delta t}{\tau}\left[f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)\right] \end{aligned} \tag{9}$$

3. COMPUTER CODE

The computer code uses the parallel computing techniques incorporated in the PETSc 2.1.0 library developed at Argonne National Laboratory, Argonne, Illinois [9] and was tested on two parallel computing clusters. The ACAD cluster has four 450 MHz Intel Pentium III processor workstations running the FreeBSD 3.2 operating system and is located at the Laboratory for Numerical Simulation and Parallel Computing in Fluid Mechanics, Center for Fundamental and Advanced Technical Research, Romanian Academy, Timi^{o}oara. The BCUM cluster has ten 1 GHz Intel Pentium III processor workstations running the Red-Hat Linux 7.2 operating system and is located at the Laboratory for Parallel Computing of the National Center for Complex Fluids Systems Engineering, a research unit recently established at the "Politehnica" University of Timi^{o}oara [10]. During the test, 500,000 iterations with time step $dt = 10^{-4}$ were done on a 10,000 nodes lattice, and the run time was recorded. Figure 1 shows the de pendence of the total run time vs. number of processors used on each cluster. Good scalability is achieved on both clusters, especially when the number of processors is increased from 1 to 4.

4. NUMERICAL RESULTS

The main characteristic of the liquid vapour systems is the phase separation, which occurs when the system temperature is lowered below the critical temperature $T_c = 1$. In the final state, the existence of two different phases: liquid phase (with higher density) and gas phase (with lower density) is clearly observed in Figure 2. When

using the CENTERED scheme, a *spurious* surface tension (Figure 2a), as well as a *spurious* velocity (Figure 3) are observed in the interface region. This feature is not present when using the MIXED scheme.

The phase coexistence diagrams recovered for both CENTERED and MIXED schemes are shown in Figure 4. One can see that the results we get using the MIXED scheme are closer to the theoretical diagram derived from the *Maxwell construction* [7]. When using the CENTERED scheme, the local velocity increases when the temperature decreases (Figure 5). Velocity profiles are dependent also on the lattice spacing dx (Figure 6). The unphysical behaviour of the CENTERED schemes appears because of a spurious term in the model continuity equation derived from Eq (8) using the procedure described in [11]:

$$\partial_t \rho + \nabla\left[\rho\mathbf{u} - \frac{1}{2}\chi c\delta x \nabla\rho\right] = 0 \qquad (10)$$

The spurious term acts in the interface region, where large density gradients are present. When using the MIXED scheme, this term is no longer present.

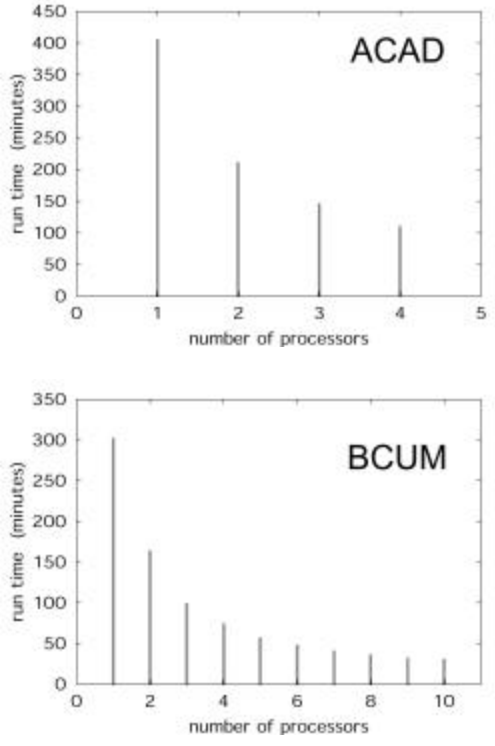
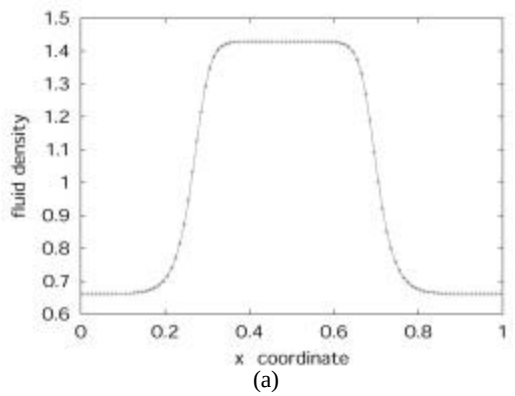
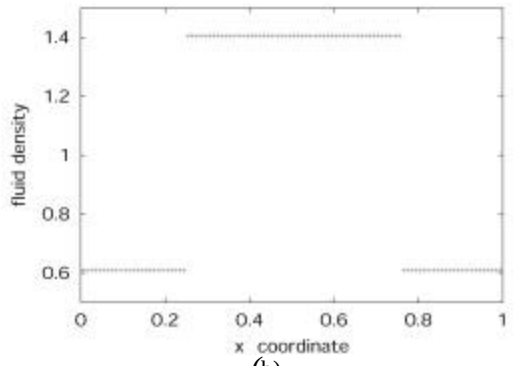


Figure 1 Run time vs. number of processors on the ACAD and BCUM clusters.



(a)



(b)

Figure 2 Density profiles obtained using the two finite difference schemes: (a)-CENTERED, (b)-MIXED at T=0.95

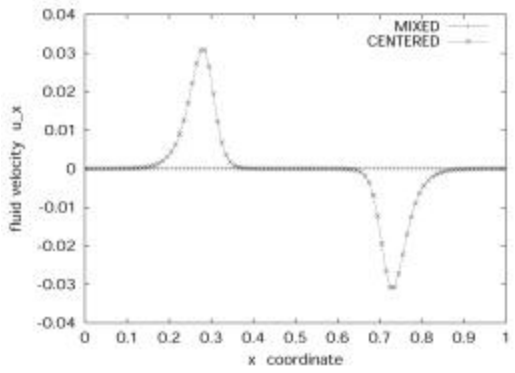


Figure 3 Velocity profiles obtained using the two finite difference schemes: MIXED, and CENTERED at T=0.95

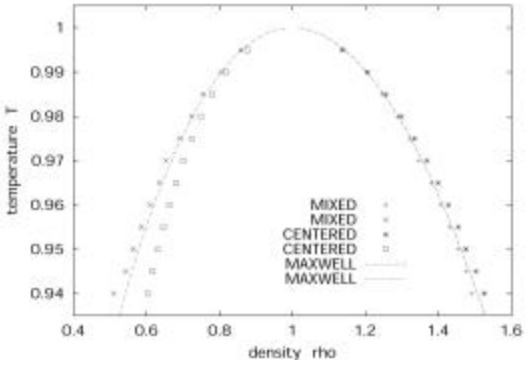


Figure 4 Phase coexistence diagram

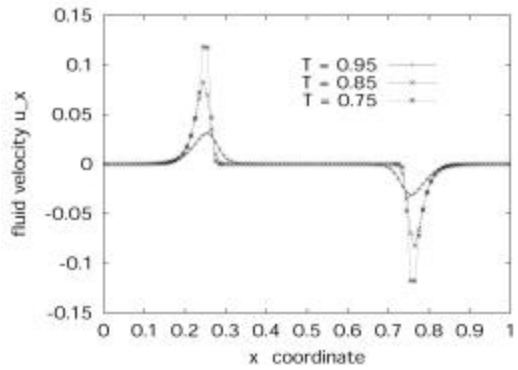


Figure 5 Velocity profiles obtained using the CENTERED scheme for different temperatures

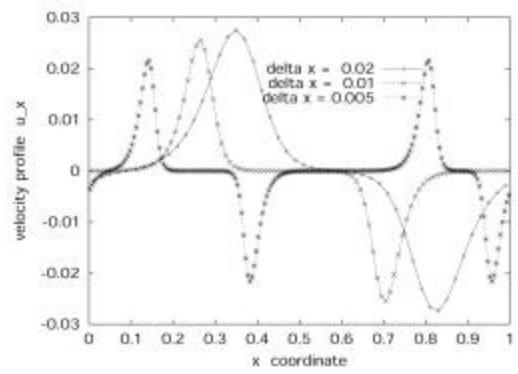


Figure 6 Velocity profiles obtained using the CENTERED scheme for different lattice spacing

5. CONCLUSIONS

In this paper we developed a finite difference lattice Boltzmann (FDLB) model for the simulation of isothermal liquid - vapour systems. Phase separation is achieved trough an interparticle force. The choice of an appropriate numerical scheme is essential to avoid spurious behaviour in the interface region.

ACKNOWLEDGEMENTS

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