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A 3D, Parallel LBM to Simulate Gravity Driven Bubbly and Slug Flows

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INTRODUCTION

Multi phase and multi component flows are ubiquitous in nature as well as in many man-made processes. Multi-phase flows typically manifest a wide variety of geometrical patterns (or flow regimes) of associated phases depending on several system conditions. These patterns include, but are not limited to, bubbly, slug, churn or annular flows. In the case of boiling this may lead to Departure from Nucleate Boiling (DNB). Simulation and identification of these flow regimes via numerical simulations is not a trivial task partly due to the need for extensive interface tracking. Consequently, analysis of multi-phase flow is still largely based on empirical formulas. In comparison with continuum approaches based on fluids equations for different phases, use of Lattice Boltzmann Method (LBM) may prove highly advantageous because of its inherent ability to incorporate particle interactions to yield phase segregation. Both, single and multi-component multiphase fluids can be simulated using this approach [1-6]. We are using LBM to address multiphase flow problems specific to nuclear engineering such as the simulation and prediction of Critical Heat Flux (CHF). Some preliminary results to simulate multi-phase flows without heat transfer are presented here.

METHODOLOGY

Lattice Boltzmann model for multiphase flow proposed by Shan and Chen (S-C model) [1] is used in this study. In this model, an interaction potential is defined for each of the component in the system. This allows the introduction of non-local interaction forces between particles at neighboring lattice sites and thereby governs the movement of particles on the lattice. To simulate single component multiphase behavior, the nature of interactions should be "attractive" among neighboring particles (of the same fluid). Whereas, interactions between different fluids (multi component flows) are "repulsive," and the magnitude of the repulsive force governs the inter-component miscibility.

In LBM, multi component fluids are simulated by introducing a separate distribution function for each of the component. The same algorithm [2, 5] is followed for each of the distribution function during temporal evolution. Multiple components interact through an interaction force between components σ and $\bar{\sigma}$ given by [5],

$$F_\sigma(\mathbf{x},t) = -G\psi_\sigma(\mathbf{x},t)\sum_a w_a \psi_{\bar{\sigma}}(\mathbf{x}+\mathbf{e_a}\Delta t,t)\mathbf{e_a}$$

where ψ is the interaction potential here taken as the macroscopic density. Effect of other potential functions, such as Lennard-Jones equivalents will be explored in the future. G is the magnitude of the interaction force which should be positive to simulate repulsive forces between the interfaces, a represents particle movement direction at any lattice point (varies from 1 to 9 in D_2Q_9 model [5, 6] and 1 to 15 in D_3Q_{15} model [5, 6]), w_a is the weighting factor, and $\mathbf{e_a}$ denotes the velocity vectors. A higher value of G leads to greater immiscibility between components and results in sharp non-diffusing interfaces.

Surface forces are computed in the same way as in the single phase for each of the component by defining surface adhesion term as [5],

$$F^\sigma_{ads}(\mathbf{x},t) = -G^\sigma_{ads}\psi_\sigma(\mathbf{x},t)\sum_a w_a s(\mathbf{x}+\mathbf{e_a}\Delta t,t)\mathbf{e_a}$$

where G^σ_{ads} is the magnitude of the surface adhesion force. Varying G^σ_{ads} results in different contact angles between the fluid and the surface. s is a Boolean vector identifying the surfaces in the domain (1, if neighbor is a surface; 0 otherwise).

Results of a 2D code, based on the S-C model, were presented earlier [2]. The code was tested successfully to simulate various problems such as the lid-driven cavity, Rayleigh-Bernard convection and instability, phase separation (spinodal decomposition), surface interactions (contact angles) and flow of immiscible fluids, etc [2]. The computer code developed earlier [2] has now been extended to three dimensions based on the D_3Q_{15} model, and has been parallelized using MPI [7]. Results reported below were obtained on a cluster of 36 processors at the Turing Facility [8]. The operating system for the Turing Cluster is Mac OS X Server, version 10.3.

RESULTS

First, results of 2D simulations to generate different flow regimes are presented. Density contours resulting from the 2D LBM simulation of bubbly flows under gravity are shown in Fig. 1. Channel is periodic in the vertical direction and bounded by walls in the horizontal direction. The domain at $t = 0$ is initialized randomly between liquid and vapor phases to yield a desired average void fraction. Depending upon the magnitude of the initial void fraction, the flow evolves to different flow regimes, such as bubby and slug flows. In the results shown (in Fig. 1), the initial void fraction for the bubbly and slug regimes is taken as 0.05 and 0.4, respectively.

Results of the 3D parallel version of the code based on D_3Q_{15} model are shown in Fig. 2. Here, a periodic rectangular channel with gravity is simulated on a 20 x 160 x 20 lattice. Results in the form of iso-surface density plots are shown in Fig. 2 (a) and (b). Here, starting from a randomly distributed void fraction, the bubbles rise and coalesce and ultimately yield a steady flow pattern.

CONCLUSIONS

Results obtained so far are very promising and show the potential of LBM to tackle multi-phase, multi-component flow simulation problems with very limited empiricism in the model. One of the first tasks in the future will be to relate the non-dimensional LBM space to the real world units. This will then allow us to, for example, verify the LBM approach by simulating a flow regime map which can then be compared with those available in the literature.

ACKNOWLEDGEMENT

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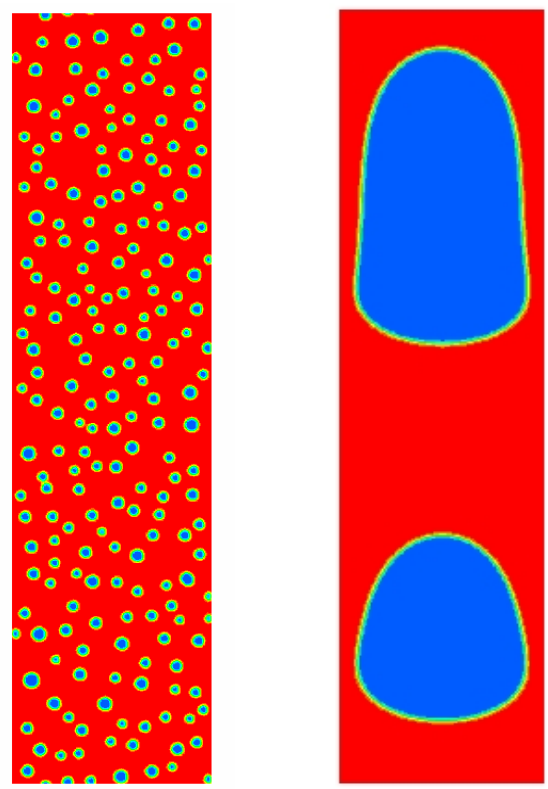
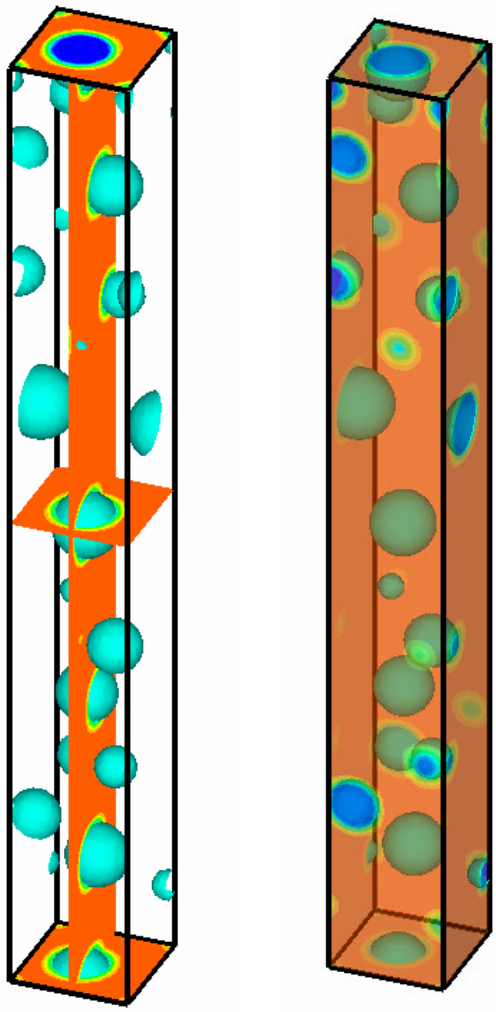
REFERENCES

1. X. SHAN and H. CHEN, "Lattice Boltzmann model for simulating flows with multiple phases and components", Physical Review E, 47 (3), 1816-1820 (1993).
2. P.K. JAIN and RIZWAN-UDDIN, "Lattice Boltzmann method (LBM) for nuclear engineering applications", Trans. ANS 96, 595-597 (2007).
3. A. TENTNER, H. CHEN and R. ZHANG, "Simulation of two-phase flow and heat transfer phenomena in a boiling water reactor using the lattice Boltzmann method", Physica A, 362, 98-104 (2006).
4. G. YADIGAROGLU, "Computational Fluid Dynamics for nuclear applications: from CFD to multi-scale CMFD," Nuclear Engineering and Design, 235, 153-164 (2005).
5. M. C. SUKOP and D. T. THORNE, JR., "Lattice Boltzmann Modeling — An Introduction for Geoscientists and Engineers", Springer-Verlag Berlin Heidelberg (2006).
6. S. SUCCI, "The Lattice Boltzmann Equation — For Fluid Dynamics and Beyond", Oxford Science Publications (2001).
7. The Message Passing Interface (MPI) standard. http://www-unix.mcs.anl.gov/mpi/
8. Turing Xserve Cluster, University of Illinois Urbana Champaign. http://www.cse.uiuc.edu/turing/



(a) (b)

Fig. 1. Density contours representing bubbly and slug flow regimes in a 2D vertical channel under gravity. Blue color depicts lower density bubbles. (a) bubbly flow, and (b) slug flow.



(a) (b)

Fig. 2. 3D LBM simulation of immiscible bubbles rising under gravity in a 20 x 160 x 20 periodic channel. Iso-surfaces with blue color representing lower density bubbles are shown. (a) iso-surface and sliced view, and (b) solid view