



A LATTICE BOLTZMANN METHOD FOR SIMULATIONS OF LIQUID-VAPOR THERMAL FLOWS

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ABSTRACT

We present a novel lattice Boltzmann method that has a capability of simulating thermodynamic multiphase flows. This approach is fully thermodynamically consistent at the macroscopic level. Using this new method, a liquid-vapor boiling process, including liquid-vapor formation and coalescence together with a full coupling of temperature, is simulated for the first time.

INTRODUCTION

After years of research, the Lattice Boltzmann Methods (LBM) has turned into a built up numerical approach in computational liquid flow (CFD). Numerous models and ex-strains have been detailed that cover an extensive variety of complex liquids and streams. Moreover, LBM has been reached out to incorporate turbulence models that have just had an immediate and generous effect on building applications.

Among numerous attractive LBM highlights, for example, effortlessness, parallelizability, and vigor in managing complex limit conditions, one perceived favorable position is its ability of reenacting liquid streams with different stages. The center instrument in LBM displaying of multiphase streams is its infinitesimal level acknowledgment of non-perfect gas conditions of state. Therefore, at sufficiently low temperature and legitimate weight, fluid vapor like first request stage advances are suddenly produced. There is no compelling reason to expressly following the interfaces between immiscible stages. Moreover, dissimilar to static measurable physical models, LBM likewise contains the energy preservation, so air pockets and fluid beads are framed alongside liquid hydrodynamic procedures. The achievement and effortlessness of LBM for multiphase streams has prompted different applications that incorporate recreations of oil-water blends through permeable media, Rayleigh-Taylor issues, and some more. Then again, there is a urgent missing piece. That is, so far all the current multiphase LBM models are constrained to administrations in which the temperature progression is either irrelevant or its launch on stream is insignificant. This constraint, alongside the general inaccessibility in CFD, has kept us from managing an imperative class of streams, in particular multiphase streams including solid couplings with thermodynamics. Particular cases of such sort of streams extend from the normal water bubbling procedures to warm atomic reactor applications. Consequently from both crucial and handy purpose of perspectives, expansions of the current CFD and LBM strategies to recreation of warm multiphase streams is critical. The LBM is initially advanced from cross section gas models obeying major preservation laws and symmetries. Presently it has additionally been appeared to be deliberately resultant from the continuum Boltzmann condition.

The most commonly known lattice Boltzmann equation (LBE) has the following form (adopting the lattice unit's convention in which $\Delta t = \Delta x = 1$),

$$f_i(\mathbf{x} + \hat{c}_i, t + 1) - f_i(\mathbf{x}, t) = C_i, \quad (1)$$

where time t takes on only positive integer values, and the particle velocity takes on a finite set of discrete vector values (speeds), $\{c_i; i = 0, \dots, b\}$. These speeds form links among nodes on a given lattice. The collision term on the right hand side of eqn. (1) now often uses the so called Bhatnagar-Gross-Krook (BGK) approximation.

$$C_i = -\frac{f_i - f_i^{eq}}{\tau}, \quad (2)$$

Having a single relaxation time parameter, τ . Here, f_i^{eq} is the local equilibrium distribution Function that has an appropriately prescribed functional dependence on the local hydrodynamic properties. The basic hydrodynamic quantities, such as fluid density ρ and velocity \mathbf{U} , are obtained through simple moment summations,

$$\begin{aligned} \rho(\mathbf{x}, t) &= \sum_i f_i(\mathbf{x}, t), \\ \rho \mathbf{u}(\mathbf{x}, t) &= \sum_i \hat{c}_i f_i(\mathbf{x}, t). \end{aligned} \quad (3)$$

In addition, one can also define a fluid temperature T from,

$$\rho \frac{D}{2} T(\mathbf{x}, t) = \sum_i \frac{1}{2} (\hat{c}_i - \mathbf{u}(\mathbf{x}, t))^2 f_i(\mathbf{x}, t), \quad (4)$$

Where D is the dimension of the momentum space of the discrete lattice velocities. It has been theoretically shown that the hydrodynamic behavior produced from LBE obeys the Navier Stokes fluid dynamics at a long wave-length and low frequency limit. The resulting equation of state is that of an ideal gas fluid, namely the pressure p obeys a linear relation with density and temperature,

$$p = \rho T. \quad (5)$$

The kinematic viscosity of the fluid is related to the relaxation parameter by

$$\nu = \left(\tau - \frac{1}{2}\right) T. \quad (6)$$

LBM has been extended to simulations of multiphase flows. The key step is to introduce an additional term, $f_i(\mathbf{X}, t)$ on the right hand side of eqn.(1), to represent a Body-force. This force term is self-consistently generated by the neighboring distribution functions around each lattice site, and it does not either violate the local mass conservation nor the global momentum conservation. However, the local momentum is altered by an amount,

$$\mathbf{F}(\mathbf{x}, t) = \sum_i \hat{c}_i \Delta f_i(\mathbf{x}, t). \quad (7)$$

The appearance of the body compel term can be physically, in a mean-field sense, credited to a non-nearby interfacial potential U among the particles. The presence of such an associating potential is the basic instrument in the non-perfect gas kind of liquids. Subsequently with a reasonable decision of U , unconstrained stage partitions can be created, and one can utilize it helpfully to numerically consider multiphase stream wonders. As the years progressed, there have been numerous advances in LBM models for multiphase streams. Then again, as pointed out toward the starting, all the current endeavors are

restricted to isothermal (or "a-warm") circumstances in which the progression of temperature in the liquid is smothered. That is, T is either expected a steady or, best case scenario, an endorsed capacity of room (or time).

The early modeling elements were first depicted by the metaphors of simple, equilateral triangles either pointing up, in order to escape like air or fire, or down, to rest like water or earth.

Later PlatoKanki and Iuchi 1973 Since the 1970s the Boltzmann equation has been connected to kinetic theory through comprehending the distribution function to get the macroscopic flow field. In order to fathom Boltzmann equation, the full distribution function of each microscopic particle should be fathomed, which confounds the calculation process.

Bird 1994 There are numerous other methods presenting the flow field from the material science of flow process as opposed to unraveling the Boltzmann Equation directly. Direct Simulation Monte-Carlo (DSMC) is the most celebrated among those methods.

Kadanoff 1986 By ignoring the microscopic subtle elements in molecular dynamics, which has trivial impact in macroscopic dynamics, one improves the kinetic equation. The Lattice Gas Automata (LG) has been produced since 1970s, which is considered as a rearranged and invented molecular dynamic model.

McNamara and Zanetti 1988 replace the particle control of Boolean variables with single-particle distribution functions of real variables and disregard singular particle movement and particle-particle correlations in the kinetic equations. This is the development which represents the birth of Lattice Boltzmann method.

Swift et al. (1995, 1996) Simulation of multiphase and multi component flows is important in numerous engineering applications, including flow through porous media, covering flow, bubbling dynamics, and dendrite formation. There are several popular Lattice Boltzmann (LB) techniques for the examination of multiphase flows, three of which are the methods and free energy approach by All three methods have been contemplated broadly with their unmistakable focal points. Out of the three, the method of Gunstensen (1991) is the most established and easiest technique which can prescribe the interfacial dynamics by preferentially redistributing the single-particle probability functions in the direction of the normal color gradient.

In this paper, we present an extension of multiphase LBM to include the full thermodynamic process.

The most natural extension in LBM for thermodynamics has been to present a con-served vitality level of flexibility. This is moderately clear for the perfect gas kind of models in which just point savvy impacts are included and just motor vitality is considered. At the point when a sufficient number of molecule speeds is utilized, one can hypothetically demonstrate that LBM prompts the right full arrangement of thermo hydrodynamic conditions of a perfect gas liquid. Lamentably, other than being extensively more costly computationally than the isothermal LB models, such an approach can't be effortlessly summed up to multiphase thermodynamic streams. The most evident hindrance is the difficulty in following the vitality development while keeping up add up to vitality preservation: For a non-perfect gas framework, the aggregate vitality additionally contains a communicating vitality part that is a component of the relative positions among the particles. Without add up to vitality protection, a temperature variable can't be characterized completely self-reliably at the infinitesimal level. Also, it has been demonstrated that, not at all like the isothermal models, a LBE with a vitality level of opportunity does not ensure a worldwide H - hypothesis. As a result, the framework can show essentially less steadiness. Other unwanted highlights in this immediate approach incorporate 1) difficulty in changing Prandtl number an incentive from solidarity, unless a considerable speculation to the BGK impact term is made; and 2) a fairly constrained temperature run (with the maximal suitable esteem just about double the negligible esteem), unless fundamentally more speeds are included. On account of these reasons, the advance in LBM for warm multiphase streams has been fairly moderate. Here we introduce another LBM approach that can basically evade the greater part of the previously mentioned disadvantages. The basic thought can be quickly outlined: First of all, the liquid progression part (i.e., the thickness and force advancement) is spoken to by an adjusted ISOTHERMAL LBE, while the vitality development part is dictated by an extra scalar vitality transport condition. The last can be tackled either by means of a limited difference conspire or a helper LBE. Furthermore, the coupling of the two sections is through a legitimately characterized body compel term in the LBE (and the pressure and dispersal terms in the vitality condition). As we might

understand beneath, albeit adroitly rather basic, the new model creates the right full thermo hydrodynamic conditions together with a non-perfect gas condition of state.

We pick a typical isothermal LBE (e.g., D3Q19,) as a beginning premise. As examined before, an isothermal LBE display for liquid thickness and speed development is extensively less complex contrasted with its vitality saving partner. This is positively attractive for doing efficient liquid stream reenactments. Besides, the balance circulation in an isothermal LB display is just a component of liquid thickness and speed. The absence of temperature elements in the harmony appropriation is the key for accomplishing a higher steadiness in LBE. Having these as a top priority, it is much alluring to acquaint a plainly visible system with recoup thermodynamics. In particular, rather than letting temperature to impact the harmony circulations in a LB framework, the thermodynamic effect is gotten by means of a temperature-subordinate body-constrain. Because of the “external” nature of the coupling, the LB system and its equilibrium property remain to be microscopically isothermal. Nonetheless, as explained below, this alternative way of coupling achieves the desired thermodynamics at the macroscopic level.

Ignoring the higher order contributions, the body-force term can be simply expressed as,

$$\Delta f_i(\mathbf{x}, t) = \frac{w_i}{T_0} \hat{c}_i \cdot \mathbf{F}, (\mathbf{x}, t) \quad (8)$$

Where the constant weights w_i and T_0 are directly determined by the LBE model (e.g., D3Q19;, in which $T_0 = 1/3$). One can easily verify that this gives rise to eqn. (7). The global momentum conservation is preserved as long as $\mathbf{F}(\mathbf{x}, t)$ is expressed as a spatial gradient of a scalar function,

$$\mathbf{F}(\mathbf{x}, t) = -\nabla U(\mathbf{x}, t). \quad (9)$$

It is straightforward to implement this condition in a discrete space by proper finite-difference procedures. Based on the consideration for higher order isometry in surface tension, we choose (for D3Q19) the following specific form,

$$\nabla U(\mathbf{x}, t) \approx \sum_i \frac{D}{bc_i^2} \hat{c}_i U(\mathbf{x} + \hat{c}_i, t) \quad (10)$$

With the additional body-force term, one can easily recognize that the overall effective pressure in the resulting fluid momentum equation has become,

$$p = \rho T_0 + U \quad (11)$$

Where the first term is a result of the isothermal LBM. From (11), one can obtain any form of equation of state, $p = p(\rho, T)$, simply by making a corresponding choice for U ,

$$U(\mathbf{x}, t) = p(\rho(\mathbf{x}, t), T(\mathbf{x}, t)) - \rho(\mathbf{x}, t)T_0. \quad (12)$$

The above quantity is determined once the neighborhood estimations of $\rho(\mathbf{x}, t)$ and $T(\mathbf{x}, t)$ are given. Clearly the subsequent liquid is never again isothermal if the temperature $T(\mathbf{x}, t)$ changes. As such, on account of the naturally visible method for coupling, the subsequent liquid progression is never again isothermal. Likewise, with the high adaptability of picking the condition of express, this approach can be connected to reproduction of non-perfect gas liquids and multiphase streams. Without a doubt, we affirmed this essential component through an arrangement of spinodal disintegration tests in light of a Van de Waals gas demonstrate (Carnahan-Starling condition of state). Like the other multiphase LBM, an unconstrained stage partition process is very much seen at sufficiently low temperature esteems.

The evolution of the temperature $T(\mathbf{x}, t)$ in this new approach is obtained from solving a supplemental scalar energy transport equation,

$$\rho(\partial_t + \mathbf{u} \cdot \nabla)e = -p\nabla \cdot \mathbf{u} + \nabla \cdot \kappa \nabla T + \Psi \quad (13)$$

Where $e = c_v T$ is the internal energy, and c_v is the specific heat at constant volume of the fluid. The overall pressure p is defined by the equation of state (11), and κ is the heat conductivity that can be specified flexibly. The term Ψ represents the viscous dissipation of flow and the contribution of surface tension. The energy evolution equation (13) is a standard macroscopic description for thermal fluids. The computation of an isothermal LB model along with a scalar energy equation is considerably less expensive than any microscopic attempts: for it neither requires many particle speeds nor complicated tracking of the energy evolution. Moreover, the difficulties in stability and Prandtl number associated with the original thermal LBM are not issues in this approach. Solving a scalar transport equation is rather straightforward. There are many finite-difference schemes for accurately and efficiently solving the scalar transport equation. In our particular simulations, we have used an extended Lax-Wendroff scheme. The combination of eqns. (1)-(3), (8)-(10), and (12)-(13) forms the new LBM approach for modeling multiphase thermodynamic fluid flows. The thermal boundary condition can be realized via standard numerical procedures so that,

$$\kappa \hat{n} \cdot \nabla T|_w = q, \quad (14)$$

With a prescribed heat flux q , that can either be fixed or a function of local properties in order to achieve a fixed wall temperature. The unit vector \hat{n} denotes the surface normal direction.

There is one more imperative element in this model worth bringing up. That is, the new approach maintains a strategic distance from the major restriction on the temperature extend that has obliged the other warm LB models. Notice the temperature just shows up in the body-constrain term in an angle work shape. Henceforth, not at all like that for balance distribution capacities, there is no total upper or lower bound on the temperature esteems aside from that it ought not change too quickly over a given determination scale. Also, there is clearly no total bound on temperature in the vitality condition.

In view of the above discussions, one can understand that the new LB demonstrates produces a completely perceptibly consistent portrayal for thermodynamic streams including summed up conditions of state. Subsequently, this approach offers a helpful and efficient numerical apparatus for concentrate warm multiphase flow problems.

Here we also exhibit computational consequences of a typical multiphase thermodynamic stream simulation with the new LB approach. In particular, a fluid vapor boiling process involving Rayleigh-Benard like convections, phase changes, together with a mind boggling temperature dynamics is simulated effectively, albeit qualitative. Although representative of an extensive variety of important applications, boiling stream issues have gotten little accomplishment from CFD in general. Subsequently, it is important that the new approach can demonstrate such a fundamental capability.

The Rayleigh-Benard convection process has been broadly utilized as a benchmark for many liquid computations. It is the most straightforward representation of a boiling marvel in which an intricate buoyancy-driven convection process happens at various values of the Rayleigh number. Then again, most of the boiling forms happen in nature also involve developments of various thermodynamic phases. That is, other than thermal convection, the liquid under goes a phase transition process in which fluid beads and vapor bubbles are generated. The most evident practical examples include the common water boiling in a pot.

We choose a standard Rayleigh-Benard setup, in which both the upper and the lower solid plates obey no-slip boundary conditions, while the horizontal boundary condition is periodic. To achieve more stable and second-order accurate numerical results, we have also applied the new scheme to the modified LB discretization formulation of He et al. As discussed above, the Carnahan-Starling equation of state is used here for convenience. The mean density value $\rho = 1.36\rho_c$. The temperature on the upper wall is fixed at $T_u = 0.795T_c$. While on the lower wall $T_l = 0.954T_c$. Here $T_c (= 0.55$ in lattice units for the decision of the model) is the critical temperature for formation of two phases. The initial temperature is set to be linearly distributed between the two plates and is consistent with their temperature boundary conditions. The simulation volume is $L \times H = 256 \times 128$ matrix points. The gravity value $g = 5 \times 10^{-6}$ (lattice units) is utilized. Keeping in mind the end goal to avoid unnecessary complications, a weak surface strain effect is also applied in the LBM stream simulation, with the goal that the surface pressure commitment to the vitality advancement can in this way be dismissed. Specifically, we pick the surface strain coefficient σ to be 0.01 for these simulations. The kinematic viscosity and the Prandtl number are set at $\nu = 0.02$ and $Pr = 10$, individually. For effortlessness, the heat capacity c_v in our multiphase stream is picked as a constant

(= 1). All the other liquid parameters are the same as in He et al. Based on the decision of these parameter values, the resulting Rayleigh number is $Ra \sim 3.0 \times 10^5$, which is considerably higher than the primary limit ($Ra_c=1708$) for a beginning of convection in the conventional single-phase Rayleigh-Benard framework.

The simulation starts from a uniform thickness distribution with one percent random fluctuations. To enhance bubble formation, small temperature fluctuations are added to the equation of state in the main lattice point layer near the base strong plate. Because of the higher temperature, a lower thickness liquid is been created that therefore leads to small vapor rises at the base plate, and then these converge with each other to shape larger size ones. The phase formation process in the simulation is combined with the convection procedure in which the more sizzling and lighter vapor phase rises while the colder and heavier fluid phase drops because of gravity. With the above decision of parameter values, such a full thermo hydrodynamic cycle apparently is able to sustain itself indefinitely. Figure 1 appear. The thickness distributions at some representative nondimensionalized (by H/g) times. One can watch the formation of two streams of rises near the base plate. One can also watch that two pairs of counter rotating convection rolls are bolted between the air pocket streams. In addition, the convection rolls are believed to pinch of the small rises from the base plate. As air pockets rise, their sizes are believed to increase somewhat. Since small air pockets move faster than large air pockets, collision and coalescence often happen among them. Figure 2 indicates streamlines of the speed field at time 39.5, from which one can clearly observe the two pairs of counter rotating convection rolls. Figure 3 delineates the corresponding temperature deviation from the linear distribution at the same time. Interestingly, the temperature displays a non-trivial behavior: Its value apparently is relatively lower in the vapor phase domains near their interfaces. As expected physically, this marvel is expected to the $p\bar{\nabla} \cdot \mathbf{U}$ term in the vitality equation (13) associated with the volume expansion from water to vapor phases. All the above simulated phenomena are qualitatively right for a realistic two phase thermodynamic stream.

We also ran another simulation with the exact same setup as the above, aside from that the surface pressure is made ten times more grounded. As found in figure 4, just a single pair of counter rotating convection rolls is created at its asymptotic state. Different from the standard single phase Bernard convection, we see that other intrinsic properties, for example, the surface strain can also alter the thermal convection characteristics in a multiphase stream.

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