# MOLECULAR DYNAMICS PERSPECTIVES ON NONIDEAL FLUID MODELS IN THE LATTICE BOLTZMANN METHOD

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**Abstract**

*Despite their widespread use, mesoscopic models for nonideal fluids have rarely been systematically validated against microscopic simulations. In this work, molecular dynamics (MD) simulations of confined fluids are mapped onto a mesoscopic framework, enabling direct comparison with lattice Boltzmann (LBM) formulations. By analyzing the moments of the distribution function, we identify a force formulation that consistently reproduces the microscopic statistics and macroscopic force balance. The results show that a hybrid formulation combining pseudopotential and free-energy approaches provides the most consistent description. These findings establish a direct link between microscopic particle dynamics and mesoscopic modeling, offering practical guidance for the development and selection of LBM models for nonideal and multiphase flows.*

***Keywords:*** ***Molecular Dynamics, Lattice Boltzmann Method, Nonideal Fluids, Pseudopotential Model, Free-Energy Model, Mesoscopic Modeling, Multiphase Flows***

## 1. Introduction

The lattice Boltzmann method (LBM) has emerged as a powerful computational tool for simulating complex fluid flows, particularly in situations involving multiphase and multicomponent systems. Unlike traditional computational fluid dynamics approaches that solve the Navier-Stokes equations directly, LBM operates at a mesoscopic level, tracking the evolution of particle distribution functions on a discrete lattice . This kinetic foundation offers significant advantages for modeling nonideal fluids, including the ability to incorporate intermolecular interactions and capture interfacial phenomena.

However, a fundamental question has persisted in the field: how well do these mesoscopic models represent the actual microscopic physics? Despite the widespread adoption of LBM for nonideal fluid simulations, systematic validation against molecular dynamics (MD) simulations—which resolve individual particle trajectories based on Newton's equations of motion—has been notably absent . This gap is significant because MD simulations provide the most direct representation of fluid behavior at the molecular scale, serving as a "ground truth" against which coarse-grained models can be assessed.

Recent work by Hiroshi Otomo and Alexander J. Wagner addresses this critical gap by establishing a direct mapping between MD simulations of confined fluids and LBM formulations . By analyzing the moments of the distribution function—the statistical quantities that connect

microscopic particle motion to macroscopic observables—the authors identify force formulations that consistently reproduce microscopic statistics and macroscopic force balance . This article reviews these findings within the broader context of nonideal fluid modeling, exploring the theoretical foundations, computational implementation, and implications for future research.

## 2. Historical Background of the Study

The development of lattice Boltzmann methods for nonideal fluids has its roots in the kinetic theory of gases and the Boltzmann equation. The classical lattice Boltzmann equation for ideal gases, expressed as

$$\bar{f}(\mathbf{r} + \mathbf{c}_i \delta t, t + \delta t) - \bar{f}(\mathbf{r}, t) = \frac{\delta t}{\tau} \left( f_i^{\text{eq}} (\rho, \mathbf{u}) - \bar{f}(\mathbf{r}, t) \right) + \mathcal{F}_i(\mathbf{F})$$

represents the discrete-time evolution of particle distribution functions, where collisions drive the system toward a local equilibrium state characterized by the Maxwell-Boltzmann distribution . For ideal gases, the pressure is given by the simple equation of state $P = \rho c_s^2$, where $c_s$ is the lattice speed of sound.

The extension to nonideal fluids required the incorporation of intermolecular forces. Two main approaches emerged: the pseudopotential model introduced by Shan and Chen, and the free-energy model developed by Swift and colleagues . The pseudopotential model introduced a non-local interaction through a potential:

$$V(\mathbf{r}, \mathbf{r}^{\prime}) = G(\mathbf{r}, \mathbf{r}_1)\psi(\mathbf{r})\psi(\mathbf{r}_1)$$

where $G(\mathbf{r}, \mathbf{r}_1)$ is a Green's function and $\psi$ is an effective number density . By considering nearest-neighbor interactions, the discrete force becomes:

$$\mathbf{F} = G\psi(\mathbf{r})\sum_{i=0}^{Q-1}w_i[\mathbf{c}_i]\psi(\mathbf{r} + \mathbf{c}_i\delta t)\mathbf{c}_i$$

which changes the equation of state to $P = \rho c_s^2 + \frac{G}{2}\psi^2$ . This simple yet powerful approach has been widely adopted, but its accuracy relative to microscopic physics remained uncertain.

The free-energy approach, in contrast, derives the interaction force from the thermodynamic free-energy functional, ensuring consistency with the underlying thermodynamics. Both approaches have been successfully applied to a range of problems, from droplet dynamics to wetting phenomena, yet their systematic comparison against MD simulations has been lacking until recently .

## - 3. Need of the Study

The need for systematic validation of nonideal fluid models in LBM arises from several critical considerations. First, the choice of force formulation can significantly impact simulation accuracy, particularly for interfacial phenomena where the density gradient is large. Without

rigorous validation against a microscopic standard, selecting the appropriate model remains an empirical process guided more by tradition than by fundamental physical insight .

Second, multiscale simulations increasingly couple LBM with MD for problems spanning from molecular to continuum scales. For example, recent work has proposed coupled numerical models where MD is used near solid surfaces to capture wettability effects while LBM handles the bulk fluid flow . The success of such multiscale approaches depends critically on the consistency between the mesoscopic LBM formulation and the microscopic MD physics at the coupling interface . If the LBM model does not reproduce the same thermodynamics and force balance as the MD simulation, the coupling will introduce unphysical artifacts .

Third, the development of hybrid models combining multiple force formulations within a single LBM framework requires understanding the strengths and limitations of each approach. The finding that a hybrid formulation—combining pseudopotential and free-energy approaches—provides the most consistent description of microscopic physics is a significant insight that can guide future model development .

Fourth, the broader scientific community needs practical guidance for selecting and implementing LBM models for nonideal flows. As applications expand into areas such as microfluidics, biomedical engineering, and energy technologies, the demand for reliable, validated simulation tools continues to grow.

## 4. Objectives

The objectives of this study are as follows:

1. To review the theoretical foundations of the lattice Boltzmann method for nonideal fluids, including the kinetic framework, force formulations, and their connection to thermodynamics.
2. To examine the methodology for mapping molecular dynamics simulations of confined fluids onto a mesoscopic framework, enabling direct comparison with LBM formulations.
3. To analyze the moments of the distribution function as a diagnostic tool for assessing the consistency between MD and LBM simulations.

4. To identify the force formulation that most consistently reproduces microscopic statistics and macroscopic force balance.
5. To evaluate the hybrid pseudopotential and free-energy formulation and its advantages over pure formulations.
6. To discuss the implications of these findings for the development and selection of LBM models for nonideal and multiphase flows.

7. To propose future research directions for establishing a direct link between microscopic particle dynamics and mesoscopic modeling.

## 5. Theoretical Framework for Nonideal Fluid Modeling

### 5.1 The Kinetic Foundation

The lattice Boltzmann method is rooted in the Boltzmann equation, which describes the evolution of the single-particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$ in phase space. For nonideal fluids, the kinetic equation can be written in a generalized BGK form:

$$\partial_t f + \mathbf{v} \cdot \nabla f = -\frac{1}{\tau} \left( f - f^{\text{eq}} \right) - \frac{1}{\rho} \frac{\partial f^{\text{eq}}}{\partial \mathbf{u}} \cdot \mathbf{F}_{\text{nloc}}$$

where $\mathbf{F}_{\text{nloc}}$ represents the nonlocal force arising from intermolecular interactions . This framework defines a family of kinetic models with $P_0$ and $\mathbf{F}$ as tunable parameters to recover the hydrodynamics of interest . The kinematic viscosity is given by $\nu = \tau c_s^2$ for the BGK model of an ideal gas.

### 5.2 Pseudopotential Model

The pseudopotential model, also known as the Shan-Chen model, introduces fluid-fluid interactions through a pseudo-potential $\psi(\rho)$. The interaction force is computed as:

$$\mathbf{F}(\mathbf{r}) = -G\psi(\mathbf{r})\sum_i w_i \psi(\mathbf{r} + \mathbf{c}_i \delta t) \mathbf{c}_i$$

where $G$ is the interaction strength parameter. For a suitable choice of $\psi$ and $G$, the model can produce a nonideal equation of state and support phase separation. The pressure tensor derived from this model is:

$$P_{\alpha\beta} = \rho c_s^2 \delta_{\alpha\beta} + \frac{G}{2}\psi^2 \delta_{\alpha\beta}$$

While simple to implement, the pseudopotential model can suffer from thermodynamic inconsistency, as the force is not derived from a free-energy functional .

### 5.3 Free-Energy Model

The free-energy model derives the interaction force from the Helmholtz free-energy functional:

$$\mathcal{F} = \int \left[ \psi_{\text{bulk}}(\rho) + \frac{\kappa}{2}(\nabla\rho)^2 \right] d\mathbf{r}$$

where $\psi_{\text{bulk}}$ is the bulk free-energy density and $\kappa$ is a parameter controlling the surface tension. The chemical potential is $\mu = \mu_0 - \kappa \nabla^2 \rho$, and the force is $\mathbf{F} = -\rho \nabla \mu$. This approach ensures thermodynamic consistency and provides a well-defined surface tension, but requires more complex discretization .

### 5.4 Hybrid Formulation

The hybrid formulation identified by Otomo and Wagner combines elements of both approaches. By constructing the force from a combination of pseudopotential and free-energy contributions, this hybrid model achieves consistency with MD simulations while retaining computational

efficiency . The specific form of the hybrid force was determined by analyzing the moments of the MD distribution function, which provide the link between microscopic correlations and macroscopic forces .

## 6. Mapping Molecular Dynamics to Mesoscopic Framework

### 6.1 MD Simulation of Confined Fluids

The validation approach employed by Otomo and Wagner involves simulating a confined fluid using molecular dynamics . The confined geometry is essential because it allows the direct computation of forces through pressure imbalance or density gradients near solid walls. The MD simulation provides a complete microscopic description of the fluid, including particle positions, velocities, and forces.

### 6.2 Moment Analysis

The bridge between MD and LBM is established through the moments of the distribution function. The zeroth moment gives density:

$$\rho = \int f \, d\mathbf{v}$$ the first moment gives momentum:

$$\rho \mathbf{u} = \int f \mathbf{v} \, d\mathbf{v}$$

and higher moments relate to stresses, heat fluxes, and other macroscopic quantities . In MD, these moments can be computed directly from particle trajectories using ensemble averaging. In LBM, the moments are determined by the distribution function evolution.

By comparing the moments obtained from MD simulations with those predicted by various LBM force formulations, Otomo and Wagner identified which formulation most faithfully reproduces the microscopic behavior .

### 6.3 Force Balance and Thermodynamic Consistency

A key aspect of the validation is the macroscopic force balance. For a confined fluid at equilibrium, the pressure gradient is balanced by the interaction force. The force formulation must reproduce the correct equation of state and density profile. The hybrid pseudopotential-free-energy formulation was found to provide the most consistent description, capturing both the microscopic statistics and the macroscopic force balance .

## 7. Implications for LBM Model Development

### 7.1 Practical Guidance for Model Selection

The findings of Otomo and Wagner provide practical guidance for the development and selection of LBM models for nonideal and multiphase flows . Researchers can now choose force formulations based on validation against microscopic simulations rather than empirical performance alone. The hybrid formulation emerges as a robust choice that balances thermodynamic consistency with computational efficiency.

### 7.2 Multi-Scale Coupling

The establishment of a direct link between microscopic particle dynamics and mesoscopic modeling has significant implications for multiscale simulations. Coupled MD-LBM models,

where MD is used near solid surfaces to capture molecular-scale effects and LBM handles bulk fluid flow, require consistency between the models at the coupling interface . The validated hybrid LBM formulation provides a reliable mesoscopic model that can be coupled with MD simulations .

### 7.3 Digital Twins and Machine Learning

The systematic mapping between MD and LBM opens opportunities for integrating machine learning approaches into fluid modeling. By training ML models on the relationship between microscopic configurations and mesoscopic forces, it may be possible to develop even more accurate surrogate models that combine the fidelity of MD with the efficiency of LBM.

## 8. Future Directions

The work of Otomo and Wagner opens several avenues for future research. First, extending the validation to dynamic flows—beyond the confined equilibrium systems studied initially—would strengthen the conclusions. Second, applying the moment-analysis framework to other LBM formulations, including those for multicomponent fluids and thermal flows, would broaden the impact .

Third, the development of automated tools for performing the mapping from MD to LBM would make the validation approach accessible to a wider research community. Fourth, the integration of these validated LBM models with machine learning for inverse problems and design optimization holds promise for accelerating engineering applications.

## 9. Conclusion

The systematic validation of nonideal fluid models in the lattice Boltzmann method against molecular dynamics simulations represents a significant advance in the field. By analyzing the moments of the distribution function, Otomo and Wagner have established a direct link between microscopic particle dynamics and mesoscopic modeling . The hybrid formulation combining pseudopotential and free-energy approaches emerges as the most consistent description, reproducing both microscopic statistics and macroscopic force balance.

These findings provide practical guidance for the development and selection of LBM models for nonideal and multiphase flows, enabling researchers to choose formulations based on validation against microscopic simulations rather than empirical performance alone. The implications extend to multiscale modeling, digital twin development, and the integration of machine learning with fluid dynamics. As the field continues to evolve, the link between MD and LBM will serve as a cornerstone for developing more accurate and reliable computational tools for complex fluid flows.

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