Variable-Property Lattice Boltzmann Flux Solver (Postprint)

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Abstract

This paper proposes a lattice-Boltzmann flux solver that considers the variation of fluid thermophysical properties. This solver can capture the effects of variations in fluid thermophysical properties on flow and heat transfer, while retaining the inherent advantages of the conventional lattice-Boltzmann method and overcoming drawbacks in aspects such as mesh generation and boundary condition treatment. This study employs this solver to simulate natural convection driven by temperature difference in a concentric annular cavity, discusses the flow and heat transfer characteristics under different temperature difference conditions, and analyzes the influence of property variations. The results show that the constant-property solution underestimates the heat transfer performance of heat exchange equipment, and furthermore, the larger the Ra number, the more significant the deviation.

Full Text

A Variable Property-based Lattice Boltzmann Flux Solver

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Abstract

A variable property-based lattice Boltzmann flux solver is proposed in the present paper. This solver is capable of capturing the effects of variation in fluid properties on flow and heat transfer characteristics. It retains the inherent advantages of conventional lattice Boltzmann method and overcomes many drawbacks such as the difficulty in using non-uniform meshes and the inconvenience of dealing with boundary conditions. In this paper, natural convection induced by a radial temperature difference in a horizontal concentric annulus is simulated using the solver, the flow and heat transfer characteristics obtained under different temperature difference conditions are studied, and variable property effects are discussed. It is found that the commonly-used constant property solution underestimates the heat transfer performance of heat exchangers, and the deviation from the variable property solution becomes increasingly notable with the increase of the Rayleigh number.

Key words: lattice Boltzmann method; lattice Boltzmann flux solver; variable property effects; natural convection

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The lattice Boltzmann method (LBM) is based on mesoscopic kinetic theory, featuring a clear physical picture of the evolution process, simple computation, easy programming, and local calculations with excellent parallelism and scalability. These characteristics provide unique advantages for simulating large-scale complex nonlinear flow problems, and LBM has been successfully applied to various complex flow problems [1-7], such as engineering heat and mass transfer, turbulence, multi-component flows, multiphase flows, and interfacial dynamics. In recent years, Shu et al. [8-9] proposed a lattice Boltzmann flux solver (LBFS) and extended its application to numerical investigations of flow and heat transfer in single-phase and multiphase fluids [10-12]. In LBFS, the macroscopic differential equations obtained through Chapman-Enskog analysis of the lattice Boltzmann equation are discretized using the finite volume method, and numerical fluxes at cell interfaces are estimated using local solutions of the Boltzmann equation. Detailed introductions to LBFS can be found in reference [8].

The influence of variable properties has been a focal point of theoretical and numerical research for decades. Existing studies have shown that temperature-dependent fluid properties significantly affect flow instability [13-16] and cannot be ignored in their impact on heat transfer performance [17-24]. However, studies employing LBM for such problems [25-26] are relatively rare and have been limited to uniform grids. This paper extends LBFS to numerical investigations of variable property fluid flow and heat transfer processes. Four key aspects of the variable property LBFS should be emphasized. First, variations in fluid viscosity, thermal conductivity, specific heat capacity, and density in the body force with temperature are considered. Second, non-uniform meshes can be conveniently employed. Third, storage requirements are minimal, as only equilibrium distribution functions need to be stored. Fourth, the method is universal, as the body force terms in the equations and additional terms introduced by property variations do not affect the numerical flux estimation process. Recently, the authors proposed an algorithm that simultaneously considers fluid density variation (VPLBFS), with detailed descriptions and systematic validation provided in reference [27].

1 Variable Property Lattice Boltzmann Flux Solver

1.1 Macroscopic Governing Equations

For variable property fluid flow and heat transfer problems, neglecting viscous dissipation and compression work, the governing equations can be written as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{1}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot [\mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \mathbf{F} \tag{2}$$

$$\frac{\partial (\rho C_p T)}{\partial t} + \nabla \cdot (\rho C_p T \mathbf{u}) = \nabla \cdot (\kappa \nabla T) \tag{3}$$

where μ, κ, and C_p are temperature-dependent functions representing fluid viscosity, thermal conductivity, and specific heat capacity, respectively, and $\mathbf{F}$ is the body force term. In this study, only the fluid density appearing in the body force term is treated as a temperature-dependent function.

1.2 Standard LBE and Multi-scale Chapman-Enskog Analysis

Similar to constant property fluids, the standard lattice Boltzmann equation (LBE) for variable property fluids can also be written in the form of equation (4):

$$f_\alpha(\mathbf{r} + \mathbf{e}_\alpha \delta_t, t + \delta_t) - f_\alpha(\mathbf{r}, t) = -\frac{1}{\tau}[f_\alpha(\mathbf{r}, t) - f_\alpha^{eq}(\mathbf{r}, t)], \quad \alpha = 0, 1, \dots, N \tag{4}$$

where $\mathbf{r}$ is the spatial coordinate, δ_t is the time step equal to the lattice spacing δ_x, $\mathbf{e}_\alpha$ is the particle velocity in direction α, N is the number of discrete velocities, τ is the relaxation time, f_α is the density distribution function in direction α, and f_α^{eq} is the corresponding equilibrium distribution function with the form:

$$f_\alpha^{eq}(\mathbf{r}, t) = \omega_\alpha \rho \left[1 + \frac{\mathbf{e}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c_s^4} - \frac{|\mathbf{u}|^2}{2c_s^2}\right] \tag{5}$$

where ω_α are weighting coefficients and c_s is the speed of sound. The values of ω_α and c_s depend on the chosen lattice model. For two-dimensional problems, the most commonly used model is D2Q9, with a schematic shown in [Figure 1: see original paper]. The discrete velocities for the D2Q9 model are:

$$\mathbf{e}_\alpha = \begin{cases} (0, 0), & \alpha = 0 \\ c[\cos((\alpha - 1)\pi/2), \sin((\alpha - 1)\pi/2)], & \alpha = 1, 2, 3, 4 \\ \sqrt{2}c[\cos((2\alpha - 5)\pi/4), \sin((2\alpha - 5)\pi/4)], & \alpha = 5, 6, 7, 8 \end{cases} \tag{6}$$

where $c = \delta_x/\delta_t$. For the D2Q9 model, the speed of sound is $c_s = c/\sqrt{3}$, and the weighting coefficients are $\omega_0 = 4/9$, $\omega_{1,2,3,4} = 1/9$, and $\omega_{5,6,7,8} = 1/36$. The distribution functions satisfy the conservation laws:

$$\sum_{\alpha=0}^{8} f_\alpha = \sum_{\alpha=0}^{8} f_\alpha^{eq} = \rho, \quad \sum_{\alpha=0}^{8} \mathbf{e}_\alpha f_\alpha = \sum_{\alpha=0}^{8} \mathbf{e}_\alpha f_\alpha^{eq} = \rho\mathbf{u} \tag{7-8}$$

Performing a Taylor expansion of equation (4) yields:

$$\delta_t \left(\frac{\partial}{\partial t} + \mathbf{e}_\alpha \cdot \nabla\right) f_\alpha + \frac{\delta_t^2}{2} \left(\frac{\partial}{\partial t} + \mathbf{e}_\alpha \cdot \nabla\right)^2 f_\alpha = -\frac{1}{\tau}(f_\alpha - f_\alpha^{eq}) + O(\delta_t^3) \tag{9}$$

In the multi-scale Chapman-Enskog analysis, the distribution function f_α and its derivatives are expanded as:

$$f_\alpha = f_\alpha^{(0)} + \varepsilon f_\alpha^{(1)} + \varepsilon^2 f_\alpha^{(2)} \tag{10a}$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \varepsilon \frac{\partial}{\partial t_1} \tag{10b}$$

$$\nabla = \varepsilon \nabla_1 \tag{10c}$$

where ε is a small parameter proportional to the Knudsen number. Substituting equation (10) into equation (9) and rearranging yields the conservation law:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\mathbf{u}) = 0 \tag{11}$$

and the macroscopic momentum equation:

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla \cdot \quad = 0 \tag{12}$$

where the stress tensor   is given by:

$$= \sum_{\alpha=0}^{8} \mathbf{e}_\alpha \mathbf{e}_\alpha \left[f_\alpha^{eq} + \left(1 - \frac{1}{2\tau}\right) f_\alpha^{(1)}\right] \tag{13}$$

The relationship between viscosity and relaxation time is:

$$\mu = \rho c_s^2 \delta_t \left(\tau - \frac{1}{2}\right) \tag{14}$$

For the temperature field, a distribution function g_α is introduced with equilibrium distribution g_α^{eq}. In this study, the D2Q4 model is employed for the temperature distribution function. After Taylor expansion and Chapman-Enskog analysis of the LBE for g_α, the conservation law (14), macroscopic control equation (15), and the relationship between thermal properties and relaxation time (16) are obtained:

$$\sum_{\alpha=0}^{3} g_\alpha = \sum_{\alpha=0}^{3} g_\alpha^{eq} = T \tag{14}$$

$$\frac{\partial T}{\partial t} + \nabla \cdot (T\mathbf{u}) = \nabla \cdot \left[\left(\tau_g - \frac{1}{2} \right) \delta_t \nabla T \right] \tag{15}$$

$$\kappa = \rho C_p c_s^2 \delta_t \left(\tau_g - \frac{1}{2} \right) \tag{16}$$

1.3 Governing Equations for Variable Property LBFS

The macroscopic control equations (11), (12), and (15) derived from the standard LBE differ from the governing equations (1)-(3) for variable property natural convection. To recover equations (1)-(3) while preserving the simple form of the lattice Boltzmann model and conservation laws, this work directly substitutes the conservation laws and relationships obtained from the standard LBE into the macroscopic control equations (1)-(3), yielding:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{E} = 0 \tag{17a}$$

$$\frac{\partial \mathbf{W}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{S} \tag{17b}$$

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \mathbf{G} = 0 \tag{17c}$$

where $\mathbf{W} = \{\rho, \rho u, \rho v, \rho C_p T\}^T$, $\mathbf{E} = \rho\mathbf{u}$, and the flux vectors $\mathbf{F}$, $\mathbf{G}$ and source term $\mathbf{S}$ are defined accordingly.

In the variable property LBFS for two-dimensional problems, equation (17) can be rewritten as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0 \tag{18a}$$

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial P_{xx}}{\partial x} + \frac{\partial P_{xy}}{\partial y} = F_x \tag{18b}$$

$$\frac{\partial (\rho v)}{\partial t} + \frac{\partial P_{yx}}{\partial x} + \frac{\partial P_{yy}}{\partial y} = F_y \tag{18c}$$

$$\frac{\partial(\rho C_p T)}{\partial t} + \frac{\partial Q_x}{\partial x} + \frac{\partial Q_y}{\partial y} = 0 \tag{18d}$$

The fluxes are calculated from:

$$P_{xx} = \sum_{\alpha=0}^{8} e_{\alpha x} e_{\alpha x} \left[f_\alpha^{eq} + \left(1 - \frac{1}{2\tau}\right) f_\alpha^{neq} \right] \tag{19a}$$

$$P_{xy} = \sum_{\alpha=0}^{8} e_{\alpha x} e_{\alpha y} \left[f_\alpha^{eq} + \left(1 - \frac{1}{2\tau}\right) f_\alpha^{neq} \right] \tag{19b}$$

$$P_{yx} = \sum_{\alpha=0}^{8} e_{\alpha y} e_{\alpha x} \left[f_\alpha^{eq} + \left(1 - \frac{1}{2\tau}\right) f_\alpha^{neq} \right] \tag{19c}$$

$$P_{yy} = \sum_{\alpha=0}^{8} e_{\alpha y} e_{\alpha y} \left[f_\alpha^{eq} + \left(1 - \frac{1}{2\tau}\right) f_\alpha^{neq} \right] \tag{19d}$$

$$Q_x = \sum_{\alpha=0}^{3} e_{\alpha x} \left[g_\alpha^{eq} + \left(1 - \frac{1}{2\tau_g}\right) g_\alpha^{neq} \right] \tag{20a}$$

$$Q_y = \sum_{\alpha=0}^{3} e_{\alpha y} \left[g_\alpha^{eq} + \left(1 - \frac{1}{2\tau_g}\right) g_\alpha^{neq} \right] \tag{20b}$$

A finite volume method is employed to solve equation (18) in the variable property LBFS. Macroscopic variables at each cell center are obtained by directly solving the discretized equations, while numerical fluxes at cell interfaces are estimated through local reconstruction using solutions from LBM. Integrating equation (18) over a control volume Ω_i yields the governing equation for the variable property LBFS:

$$\frac{d\mathbf{W}_i}{dt} = -\frac{1}{V_i} \sum_{k=1}^{M} \mathbf{R}_k S_k + \mathbf{S}_i \tag{21}$$

where V_i is the volume of control cell Ω_i, S_k is the area (length) of the k-th interface, and $\mathbf{R}_k$ is the numerical flux at the k-th interface. The specific procedure for estimating $\mathbf{R}_k$ can be found in reference [8]. After obtaining $\mathbf{R}_k$, a 4th-order Runge-Kutta method is used to solve equation (21).

2 Validation of Variable Property LBFS

To validate the reliability of the variable property LBFS, the natural convection in a square cavity from reference [21] was simulated before investigating the concentric annulus case. The cavity has adiabatic top and bottom walls, with constant-temperature hot and cold vertical walls on the left and right sides, respectively, denoted as T_h and T_c. Equation (22) defines a dimensionless temperature difference ratio θ to measure the magnitude of temperature difference:

$$\theta = \frac{T_h - T_c}{T_c} \tag{22}$$

In the three test cases, the Rayleigh number Ra is fixed at 10^5, the Prandtl number Pr is 0.71, T_c is 300K, and θ takes values of 0.0101, 0.403, and 0.8, corresponding to T_h values of 303.03K, 420.9K, and 540K, respectively. Fluid thermophysical properties—viscosity μ, specific heat capacity C_p, and thermal conductivity κ—are temperature-dependent functions adopted from reference [18], while density in the body force term uses the Boussinesq approximation.

Unlike traditional LBM, the variable property LBFS can conveniently employ non-uniform meshes and directly impose boundary conditions using macroscopic variables rather than distribution functions. For natural convection under these conditions, grid independence studies show that a 50×50 non-uniform mesh is sufficient to obtain accurate steady-state solutions. Boundary conditions are implemented by directly specifying no-slip velocity on all walls, constant temperature on the vertical walls, and adiabatic conditions on the horizontal walls. Initially, the fluid is stationary at temperature T_c.

[Figure 2: see original paper] compares steady-state solutions under different temperature difference conditions, showing streamlines and isotherms. The results demonstrate that temperature-dependent fluid properties noticeably affect both flow and temperature fields, with the influence strengthening as temperature difference increases. To quantitatively analyze the heat transfer impact, the average Nusselt number Nu on the hot left wall is calculated. [Figure 3: see original paper] shows the temporal evolution of Nu under different temperature difference conditions. When $\theta = 0.0101$, the Nu value is very close to the constant property solution, where fluid properties (μ, C_p, κ) are evaluated at temperature T_c. These qualitative results are consistent with reference [28]. In this study, the constant property solution serves as a reference for quantitative comparison to analyze variable property effects.

As temperature difference increases, the heat transfer rate gradually increases. The results shown in [Figure 2: see original paper] and [Figure 3: see original paper] agree well with reference [21], demonstrating that the variable property LBFS can effectively capture the effects of temperature-dependent fluid properties on flow and temperature fields.

3 Natural Convection in a Concentric Annulus

This section employs the variable property LBFS to simulate flow and heat transfer driven by radial temperature differences in a concentric annulus. The inner and outer radii are denoted as r_i and r_o, respectively, with an aspect ratio $R = r_o/r_i = 2.6$. The inner and outer wall temperatures are T_c and T_h. Similar to Section 2, the effects of temperature-dependent properties are discussed by comparing numerical results under different temperature difference conditions. T_c is fixed at 300K, the dimensionless temperature difference ratio θ takes values of 0.0101, 0.403, and 0.8, and the Prandtl number Pr is 0.71. Initially, the fluid is stationary at temperature T_c. No-slip velocity conditions are applied at the walls. Non-uniform grids are used in the radial direction and uniform grids in the circumferential direction.

3.1 Constant Property Solution

First, a simplified form of the variable property LBFS is used to obtain constant property solutions for natural convection in the concentric annulus, ignoring temperature dependence of viscosity, thermal conductivity, and specific heat capacity. The grid resolution is 180×40.

[Figure 4: see original paper] shows the distributions of velocity components and isotherms in the constant property solution for $Ra = 50,000$.

3.2 Effects of Variable Properties

To quantitatively analyze how property variations affect heat transfer rate, natural convection in the concentric annulus is simulated under three different θ conditions using the variable property LBFS. Fluid viscosity, thermal conductivity, and specific heat capacity are temperature-dependent functions from reference [18]. Ra and Pr are 50,000 and 0.71, respectively.

[Figure 5: see original paper] compares velocity components and isotherms under different θ conditions. Similar to the square cavity case, temperature-dependent properties noticeably affect both velocity and temperature fields, with the influence becoming more pronounced as θ increases. To quantify the heat transfer impact, the heat transfer coefficient $\kappa_{eq,o}$ on the outer cylinder is calculated. Following reference [28], $\kappa_{eq,o}$ is defined as:

$$\kappa_{eq,o} = \frac{\dot{Q}}{2\pi\kappa\theta} = \frac{1}{\ln(r_o/r_i)} \int_{r_i}^{r_o} \frac{1}{r}\frac{\partial T}{\partial r} dr \tag{23}$$

[Figure 6: see original paper] shows the temporal evolution of $\kappa_{eq,o}$ under different temperature difference conditions. When $\theta = 0.0101$, property variations are relatively small, and the difference between variable and constant property solutions is minimal, with $\kappa_{eq,o}$ slightly larger than the constant property value. As θ increases, variable property effects strengthen. At $\theta = 0.8$, the variable property $\kappa_{eq,o}$ is 15% higher than the constant property value under the same Ra and Pr conditions. This quantitative result is similar to that in the square cavity case, indicating that: (1) the commonly-used constant property solution underestimates heat transfer performance, and (2) the deviation increases with temperature difference.

3.3 Effects Under Different Rayleigh Numbers

To further analyze variable property effects, natural convection under different Ra conditions is simulated using the variable property LBFS, and the steady-state heat transfer coefficient $\kappa_{eq,o}$ on the outer cylinder is calculated. [Figure 7: see original paper] shows $\kappa_{eq,o}$ from variable property solutions at different Ra. As Ra increases, $\kappa_{eq,o}$ increases, and the influence of temperature-dependent properties becomes more significant. In other words, under the same temperature difference conditions, larger Ra leads to more pronounced variable property effects on heat transfer. This suggests that variable property effects are not sensitive to changes in equipment geometry but that neglecting temperature-dependent fluid properties in numerical calculations can lead to significant errors, particularly at large temperature differences and high Rayleigh numbers.

Conclusion

This paper proposes a variable property-based lattice Boltzmann flux solver (variable property LBFS) that retains the advantages of traditional LBM while overcoming drawbacks in mesh generation and boundary condition treatment. Numerical investigations of natural convection driven by temperature differences in a concentric annulus demonstrate that the commonly-used constant property solution underestimates heat transfer rates in thermal equipment, particularly under large temperature differences and high Rayleigh numbers.

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Note: Figure translations are in progress. See original paper for figures.