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Postprint: A Variable-Property Lattice Boltzmann Flux Solver

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Abstract

This paper presents a lattice Boltzmann flux solver that accounts for variations in fluid thermophysical properties. The solver can capture the influence of changing fluid property parameters on flow and heat transfer, preserving the inherent advantages of conventional lattice Boltzmann methods while overcoming limitations in mesh generation, boundary condition treatment, and other aspects. Using this solver, the present work simulates temperature-difference-driven natural convection in a concentric annular cavity, examines flow and heat transfer characteristics under various temperature difference conditions, and analyzes the effects of property variations. The results demonstrate that constant-property solutions underestimate the heat transfer performance of thermal equipment, with the deviation becoming more pronounced at higher Rayleigh numbers (Ra).

Full Text

Preamble

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 the variation in fluid properties on flow and heat transfer characteristics. It retains inherent advantages of conventional lattice Boltzmann method and overcomes many drawbacks such as the difficulty in using non-uniform meshes, the inconvenience

of dealing with boundary conditions, etc. In the present paper, the natural convection induced by a radial temperature difference in a horizontal concentric annulus is simulated by 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-concerned constant property solution (CPS) underestimates the heat transfer performance of heat exchangers, and the deviation of the CPS from the variable property solution becomes more and more notable with the increase of the Rayleigh number Ra .

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

The lattice Boltzmann method (LBM) is based on mesoscopic kinetic theory, featuring clear physical pictures of evolution, simple computation, easy programming, local calculations, good parallelism and scalability. It has unique advantages in simulating large-scale complex nonlinear flow problems and has been successfully applied to various complex flows [1-7], such as engineering heat and mass transfer, turbulence, multicomponent flows, multiphase flows, interfacial phenomena, chemical reactions, and combustion.

In recent years, Shu et al. [8-9] proposed a lattice Boltzmann flux solver (LBFS) and extended its application to numerical studies of single-phase fluid flow and heat transfer [10-12]. In LBFS, the conserved differential equations are obtained through Chapman-Enskog (C-E) analysis of the lattice Boltzmann equation, and then discretized using the finite volume method. The numerical fluxes at cell interfaces are estimated using local solutions of the lattice Boltzmann equation. For detailed information about LBFS, please refer to [8].

The effect of variable properties has been a hot topic in theoretical and numerical research over the past few decades. Existing studies have shown that the variation of fluid thermophysical properties with temperature significantly affects flow instability [13-16] and cannot be ignored in heat transfer performance [17-24]. However, studies using LBM to investigate such problems [25-26] are relatively rare, and they can only employ uniform grids.

This paper extends LBFS to numerical studies of variable-property fluid flow and heat transfer. Regarding the variable-property LBFS in this work, four points should be emphasized. First, it accounts for the temperature dependence of fluid viscosity, thermal conductivity, specific heat capacity, and density in the body force term. Second, it can conveniently employ non-uniform grids. Third, it requires small storage, as only the equilibrium distribution functions need to be stored. Fourth, it has good universality, as the body force term and additional terms introduced by property variations do not affect the numerical flux estimation process. Recently, the authors proposed an algorithm that can simultaneously consider fluid density variations (VPLBFS), which was described in detail and systematically validated in [27].

1 Variable Property Lattice Boltzmann Flux Solver

1.1 Macroscopic Governing Equations

For variable-property fluid flow and heat transfer problems, the governing equations can be written in the following form under the assumption of negligible viscous dissipation and compressive work:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot [\mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \rho \mathbf{f} \\ \frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) &= \nabla \cdot (\kappa \nabla T)\end{aligned}$$

In this study, fluid viscosity μ , thermal conductivity κ , and specific heat capacity c_p are all functions of temperature, \mathbf{f} is the body force, and only the fluid density appearing in the body force term is temperature-dependent.

1.2 Standard LBE and Multiscale Chapman-Enskog Analysis

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

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

where \mathbf{x} is the spatial coordinate, δ_t is the particle motion time step, equal in magnitude to the lattice size δ_x , \mathbf{e}_α is the particle velocity in the α direction of the lattice model, N is the number of particle velocities, τ is the relaxation time, f_α is the density distribution function in the α direction, and f_α^{eq} is the corresponding equilibrium distribution function with the form of equation (5):

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

where ω_α is the weighting coefficient, c_s is the sound speed, and the values of ω_α and c_s depend on the selected lattice model. For two-dimensional problems, the most commonly used lattice model is the D2Q9 model. Figure 1 [Figure 1: see original paper] shows a schematic of the D2Q9 model, where particle velocities in each direction have the form of (6):

$$\mathbf{e}_\alpha = \begin{cases} (0, 0), & \alpha = 0 \\ c[\cos[(\alpha - 1)\pi/2], \sin[(\alpha - 1)\pi/2]], & \alpha = 1, 2, 3, 4 \\ \sqrt{2}c[\cos[(2\alpha - 9)\pi/4], \sin[(2\alpha - 9)\pi/4]], & \alpha = 5, 6, 7, 8 \end{cases}$$

For the D2Q9 model, the sound speed $c_s = c/\sqrt{3}$ and $\delta_t = \delta_x/c$, with weighting coefficients $\omega_0 = 4/9$, $\omega_{1,2,3,4} = 1/9$, and $\omega_{5,6,7,8} = 1/36$.

f_α and f_α^{eq} satisfy the conservation laws (7) and (8):

$$\sum_{\alpha} f_{\alpha} = \sum_{\alpha} f_{\alpha}^{eq} = \rho$$

$$\sum_{\alpha} \mathbf{e}_{\alpha} f_{\alpha} = \sum_{\alpha} \mathbf{e}_{\alpha} f_{\alpha}^{eq} = \rho \mathbf{u}$$

Performing Taylor expansion on equation (4) yields the following equation (9):

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

For the temperature field, a distribution function g is introduced, with its equilibrium distribution function denoted as g^{eq} . In this paper, the D2Q4 model is adopted for the temperature distribution function g . After performing Taylor expansion and Chapman-Enskog analysis on the LBE satisfied by g , the conservation law (14), the macroscopic governing equation (15), and the relationship between thermophysical properties and relaxation time τ_g (16) can be obtained.

In the multiscale Chapman-Enskog analysis, the distribution function f_{α} and its partial derivatives with respect to time and space are expanded in multiple scales as follows:

$$f_{\alpha} = f_{\alpha}^{(0)} + \epsilon f_{\alpha}^{(1)} + \epsilon^2 f_{\alpha}^{(2)} + \dots$$

$$\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \dots$$

$$\nabla = \epsilon \nabla_1$$

where ϵ is a small parameter proportional to the Knudsen number.

Substituting equation (10) into equation (9) and rearranging yields the following equations (11) and (12):

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

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla \cdot \left[c_s^2 \left(\tau - \frac{1}{2} \right) \delta_t^{(1)} \right]$$

1.3 Governing Equations of Variable-Property LBFS

The macroscopic governing equations (11), (12), and (15) derived from the standard LBE differ from the governing equations (1), (2), and (3) for variable-property natural convection. To recover equations (1)-(3) while retaining the concise form of the lattice Boltzmann model and conservation laws, this paper directly substitutes the conservation laws and relationships obtained from the standard LBE into the macroscopic governing equations (1)-(3), yielding the following equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (17a)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla \cdot \mathbf{q} = -\nabla p + \nabla \cdot [\mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \rho \mathbf{f} \quad (17b)$$

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \mathbf{u} T) + \nabla \cdot \mathbf{q} = \nabla \cdot (\kappa \nabla T) \quad (17c)$$

For two-dimensional problems, equation (17) in the variable-property LBFS can be rewritten in the following form:

$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \frac{\partial \mathbf{F}_v}{\partial x} + \frac{\partial \mathbf{G}_v}{\partial y} + \mathbf{S} \quad (18)$$

where

$$\mathbf{W} = [\rho, \rho u, \rho v, \rho c_p T]^T$$

$$\mathbf{F} = [\rho u, \rho u^2 + p, \rho uv, \rho c_p u T]^T, \quad \mathbf{G} = [\rho v, \rho uv, \rho v^2 + p, \rho c_p v T]^T$$

$$\mathbf{F}_v = [0, \tau_{xx}, \tau_{xy}, q_x]^T, \quad \mathbf{G}_v = [0, \tau_{xy}, \tau_{yy}, q_y]^T$$

$$\mathbf{S} = [0, \rho f_x, \rho f_y, 0]^T - \nabla \cdot \mathbf{q}, \quad \nabla \cdot \mathbf{q} = \left[0, \frac{\partial \Pi_{xx}}{\partial x} + \frac{\partial \Pi_{xy}}{\partial y}, \frac{\partial \Pi_{xy}}{\partial x} + \frac{\partial \Pi_{yy}}{\partial y}, \frac{\partial q'_x}{\partial x} + \frac{\partial q'_y}{\partial y} \right]^T$$

In the variable-property LBFS, the finite volume method is employed to solve equation (18), where macroscopic physical quantities at each cell center are obtained by directly solving the discretized equations, and numerical fluxes at adjacent cell interfaces are estimated through local reconstruction using LBM solutions. Following the finite volume method, equation (18) is integrated over

the control volume Ω to obtain the governing equation (21) that needs to be solved in the variable-property LBFS:

$$\frac{d\mathbf{W}}{dt} = -\frac{1}{\Omega} \sum_{i=1}^{N_s} \mathbf{F}_i S_i + \mathbf{S} \quad (21)$$

where Ω is the volume of the control volume, S_i is the area (length) of the i th interface (line), and \mathbf{F}_i is the numerical flux at the i th interface (line). For specific details on estimating \mathbf{F}_i , please refer to [8]. After obtaining \mathbf{F}_i , the 4th-order Runge-Kutta method is used to obtain the numerical solution of equation (21).

2 Validation of Variable-Property LBFS

To validate the reliability of the variable-property LBFS, before simulating natural convection in a concentric annular cavity, the work in [21] was first reproduced by simulating natural convection in a square cavity. The top and bottom walls of the cavity are adiabatic, while the left and right sides are constant-temperature hot and cold walls with temperatures denoted as T_h and T_c , respectively. Equation (22) defines a dimensionless temperature difference ratio θ to measure the magnitude of temperature difference:

$$\theta = \frac{T_h - T_c}{T_c} \quad (22)$$

In the three test cases of this paper, the Rayleigh number Ra is constantly 10^5 , the Prandtl number Pr is constantly 0.71, T_c is constantly 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. The thermophysical properties of the fluid—viscosity μ , specific heat capacity c_p , and thermal conductivity κ —are all functions of temperature, with functional expressions adopted from [18]. The fluid density in the body force term still employs the Boussinesq approximation.

Figure 2 [Figure 2: see original paper] shows comparisons of steady-state solutions obtained under different temperature difference conditions, including streamlines and isotherms. As shown in Figure 2, the variation of fluid thermophysical properties has a noticeable impact on both flow and temperature fields, and this effect gradually strengthens as the temperature difference increases. To quantitatively analyze the effect of fluid thermophysical property variations on heat transfer, the average Nusselt number Nu on the left hot wall is calculated. Figure 3 [Figure 3: see original paper] shows the temporal evolution of Nu under different temperature difference conditions. As shown in Figure 3, when the temperature difference is 0.0101, Nu is very close to the constant-property solution value. As the temperature difference increases, the heat transfer rate gradually increases. The results shown in Figures 2 and 3 agree well with those

in [21], demonstrating that the variable-property LBFS can effectively capture the effects of fluid thermophysical property variations on flow and temperature fields.

Unlike traditional LBM, the variable-property LBFS can conveniently employ non-uniform grids for numerical solution, and boundary conditions can be specified directly using macroscopic physical quantities rather than through distribution functions. For natural convection in a cavity under the above conditions, the variable-property LBFS was used for solution. After grid independence verification, it was found that a 50×50 non-uniform grid is sufficient to obtain accurate steady-state solutions. Additionally, for boundary condition treatment, no-slip velocity conditions on all four walls, constant temperature conditions on the left and right walls, and adiabatic conditions on the top and bottom walls were directly specified.

3 Natural Convection in a Concentric Annular Cavity

This paper employs the variable-property LBFS to simulate flow and heat transfer processes driven by radial temperature differences in a concentric annular cavity. The inner and outer radii of the concentric annulus are denoted as r_i and r_o , respectively, with aspect ratio $R = r_o/r_i$. The inner and outer wall temperatures are denoted as T_i and T_o .

Similar to Section 2, the effect of fluid thermophysical property variations is discussed through comparisons of numerical results under different temperature difference conditions. T_c is constantly 300K, the dimensionless temperature difference ratio θ takes values of 0.0101, 0.403, and 0.8, and the Prandtl number Pr is constantly 0.71. Initially, the fluid is at rest with temperature T_c . No-slip velocity boundary conditions are adopted, with non-uniform grids in the radial direction and uniform grids in the circumferential direction.

3.1 Constant-Property Solution

First, using a simplified form of the variable-property LBFS that neglects the temperature dependence of fluid viscosity, thermal conductivity, and specific heat capacity, the constant-property solution for natural convection in the concentric annular cavity was obtained. The grid size is 180×40 . Figure 4 [Figure 4: see original paper] shows the distributions of velocity components and isotherms in the constant-property solution. The Rayleigh number $Ra = 5 \times 10^4$, and fluid property parameters such as viscosity μ , specific heat capacity c_p , and thermal conductivity κ take values at temperature T_c . These qualitative results are consistent with those in [28]. In this paper, the constant-property solution serves as a reference for quantitative comparison to analyze variable-property effects in the following sections.

3.2 Effects of Variable Properties

In this section, the variable-property LBFS is used to simulate natural convection in the concentric annular cavity under three different θ conditions. The fluid viscosity, thermal conductivity, and specific heat capacity are all functions of temperature, with functional relationships still adopted from [18]. Ra and Pr are 50000 and 0.71, respectively.

Figure 5 [Figure 5: see original paper] shows comparisons of numerical solutions under different θ conditions, including distributions of velocity components and isotherms. Similar to the case in the square cavity, variations in thermophysical properties have a noticeable impact on both velocity and temperature fields. Moreover, as the temperature difference ratio increases, the effect of property variations gradually strengthens.

To quantitatively analyze the effect of property variations on heat transfer rate, the heat transfer coefficient κ_o on the outer annulus is calculated. According to [28], κ_o can be defined in the form of (23):

$$\kappa_o = \frac{q_o R}{\kappa_c (T_i - T_o)} \quad (23)$$

Figure 6 [Figure 6: see original paper] shows the temporal evolution of κ_o under different temperature difference conditions. As shown in Figure 6, when $\theta = 0.0101$, property variations are relatively small, and the relative error between the variable-property solution and the constant-property solution is minimal, with κ_o slightly larger than that in the constant-property solution. As the temperature difference ratio increases, the effect of property variations gradually strengthens. When $\theta = 0.8$, κ_o in the variable-property solution is 15% larger than that in the constant-property solution under the same Ra and Pr conditions. This quantitative result is similar to that obtained in the square cavity.

This indicates that, on the one hand, the effect of variable properties is not sensitive to changes in equipment geometry. On the other hand, the constant-property solution obtained by neglecting fluid thermophysical property variations in numerical calculations underestimates the heat transfer performance of convective heat transfer systems, and the deviation caused by thermophysical property variations increases with larger temperature differences.

3.3 Effects of Variable Properties under Different Ra Conditions

To further analyze the effect of variable properties, this paper uses the variable-property LBFS to simulate natural convection driven by temperature differences in the concentric annular cavity under different Ra conditions, and calculates the heat transfer coefficient κ_o on the outer annulus at steady state. Figure 7 [Figure 7: see original paper] shows κ_o in the variable-property solution under different Ra . As can be seen from the figure, κ_o gradually increases with increasing

Ra , and the effect of fluid thermophysical property variations on κ_o gradually strengthens. In other words, under the same temperature difference conditions, the larger the Ra , the more significant the effect of variable properties on heat transfer.

Conclusion

This paper proposes a variable-property lattice Boltzmann flux solver (variable-property LBFS) based on fluid property variations. This solver retains the advantages of conventional LBM while overcoming many drawbacks of traditional LBM in mesh generation and boundary condition treatment. Numerical results regarding natural convection driven by temperature differences in a concentric annular cavity indicate that the commonly used constant-property solution underestimates the heat transfer rate of heat exchange equipment, particularly when temperature differences and Rayleigh numbers are relatively large.

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