Development of an immersed boundary-thermal lattice boltzmann solver for fluid-particle interaction in energy management systems

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Abstract. Computer simulations of a wide range of applications like materials processing, thermal energy storage and conversion systems, nuclear reactors, solar energy, and pollution control, etc. are of high importance in this era. In many of these applications, strong thermo-fluidic interactions between fluid and structures exist. Efficient and accurate numerical modelling of these interactions provide initial predictions of the process, but at times, it becomes challenging where complex shape of the structures is involved. To address this issue, often numerical methods that are proposed suffer lower computational accuracy and complex algorithms to capture interfacial predictions. In this paper, development, accuracy study and robustness of an in-house openMP parallelized Immersed Boundary-Thermal Lattice-Boltzmann (IB-TLB) solver are presented, which is capable of simulating complex boundary problems involving thermal interactions and accurately capture interfacial predictions. The solver showed excellent agreement with literature for a natural convection problem involving eccentrically placed stationary heated cylinder inside a cold square enclosure and forced convection around an iso-thermal circular cylinder. The numerical simulation of moving bodies is already quite a complex problem and the complexity increases further when we introduce heat transfer phenomena in it. Spatial order of accuracy test revealed, the IB-TLB algorithm exhibits first-order accuracy for velocity and temperature errors while pressure error retained second-order accuracy for moving boundary problems. It is also observed that the present algorithm can accurately predict local parameters like coefficient of pressure and Nusselt number with good accuracy and thus possesses promising potential to simulate complex moving boundary problems. The present solver will find its application in a wide range of areas such as heat exchangers, solar energy systems and chemical and food industries etc.

Keywords: Immersed boundary method, Lattice Boltzmann method, Moving boundary, Thermal management systems
1. Introduction

Numerical simulation of any physical phenomena has emerged as an effective design and research tool in recent decades that provides first-hand experience for design and development of many products. Computational fluid dynamics tools are being extensively used in numerous industries and applications like chemical and food industries, solar energy systems, electronic cooling systems, heat exchangers, materials processing, home ventilation and many more. Amongst several computational fluid dynamics tools, immersed boundary lattice Boltzmann method (IB-LBM) has emerged as a powerful tool to simulate complex fluid and heat transfer phenomena. Simulation of complex moving bodies is already quite a complex problem and the challenge increases further when we incorporate heat transfer into it. The no-slip boundary condition is conventionally incorporated using bounce-back scheme which requires particle distribution function reconstruction for newly born fluid nodes during particle motion and creates spurious force fluctuations. In most recent years, improvisation in this regard has been attempted by coupling immersed boundary method (IBM) to lattice Boltzmann method [1] [2] [3]. An extensive study of the IB-LB algorithm involving order of accuracy and robustness to simulate complex boundary problems involving thermo-fluidic interaction is not highlighted in existing literature.

In the present study, an in-house openMP parallelised immersed boundary lattice Boltzmann (IB-LB) solver is developed which is capable of simulating complex moving boundary problems involving fluid-particle interaction and heat transfer with finite accuracy. This study includes problems involving natural convection and forced convection phenomena in complex geometry which are not aligned with regular Cartesian mesh. Several studies related to order of accuracy of the solver and determination of local parameters like pressure coefficient and Nusselt number are showcased for various problems. The accurate prediction of thermo-fluidic interaction between fluid and solid sets the platform for the solver to be capable of solving numerous real life applications related to energy management systems.

2. Methodology : Immersed Boundary-Thermal Lattice Boltzmann Method

The Lattice Boltzmann Method, is a mesoscopic method that is based on lattice Boltzmann equation involving particle distribution functions. Discretized governing IB-LB equation (1) [2] is solved over Eulerian lattice points (ζ), from where information (in terms of velocity, pressure, temperature etc.) are interpolated to immersed Lagrangian points (Γ).

\[ f_i(\mathbf{x} + c_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i^{BGK} + F_i \Delta t \]  

The direct forcing term \( F_i \) in equation (1) can be expressed as [4]

\[ F_i = \left(1 - \frac{1}{2\tau_r}\right) w_i \left(\frac{c_i - \mathbf{u}}{c_s^2} + \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^2} \mathbf{c}_i\right) \cdot \mathbf{F}_b \]  

where \( \mathbf{F}_b(\mathbf{x},t) \) is the fluid body force density.

The immersed boundary thermal lattice Boltzmann equation (IB-TLB) in a uniform lattice with single relaxation time BGK collision operator can be expressed as

\[ g_i(\mathbf{x} + c_i \Delta t, t + \Delta t) = g_i(\mathbf{x}, t) + \frac{1}{\tau_g} \left(g_i^{eq}(\mathbf{x}, t) - g_i(\mathbf{x}, t)\right) + \left(1 - \frac{1}{2\tau_g}\right) Q_i \Delta t \]  

where \( Q \) is the discrete energy source function.

\[ Q_i = w_i Q \]  

\[ T(\mathbf{s}, t) = \int_{\zeta} T(\mathbf{x}, t) \delta(\mathbf{x} - \mathbf{X}(\mathbf{s}, t)) \, d\mathbf{x} \]  

The energy source density \( (Q) \) is evaluated using the boundary energy forcing term \( (Q_b) \) as

\[ Q(\mathbf{x}, t) = \int_{\Gamma} Q_b(\mathbf{s}, t) \delta(\mathbf{x} - \mathbf{X}(\mathbf{s}, t)) \, ds \]
Macroscopic internal energy can be updated as

\[ \rho e = \sum g_i + \frac{\Delta t Q}{2} \]  \hspace{1cm} (7)

The equilibrium energy density function \( g_i^\text{eq} \) and thermal boundary conditions on the computational domain are incorporated by following Liu et al. [5].

3. Results and Discussion

3.1. Natural convection in an eccentrically placed cylinder inside an enclosure

In the present subsection, a circular cylinder having diameter \( d \) is eccentrically placed inside a square enclosure of side \( L \) such that \( d=0.4L \). The cylinder's center is varied in positive y-direction, such that new location of the cylinder center and domain center is eccentric by a distance \( \delta \). The cylinder is provided constant hot temperature \( T_h \), while the domain boundaries and initial temperature of the domain are set to constant cold temperature \( T_c \). In the current simulation parameters are set as \( Pr=0.7 \) while varying Rayleigh numbers as \( Ra=10^4 \) and \( 10^5 \) for different locations of the cylinder \( \delta=0.0, 0.15L, 0.25L \).

Figure 1. Streamline (left) and isotherm (right) contours for (a) \( Ra=10^4, \delta=0.0 \), (b) \( Ra=10^4, \delta=0.25 \) and (c) \( Ra=10^5, \delta=0.0 \).

Fluid adjacent to the hot circular cylinder gradually gets warm and moves upward. It subsequently cools down and descends along the cold enclosure wall forming two symmetric free circulations in the enclosure. At \( \delta=0.0, Ra=10^4 \) (figure 1a), flow is conduction dominant and the circulation exhibits two rotating symmetric vortices. As Rayleigh number increases to \( Ra=10^5, \delta=0.0 \) (figure 1c), convection heat transfer dominates. In addition to it, development of plume at the top of the cylinder is observed owing to the stronger thermal gradient at cylinder’s top. In higher Rayleigh numbers, two inner vortices merged giving rise to a dominant flow and core of the recirculating eddies moved towards upper part of the cylinder. As the cylinder is traversed in the positive y-direction (figure 1b), merger of two vortices into one is observed. At \( Ra=10^4, \delta=0.0 \) (figure 2a), \( Nu \) at mid length of the top wall of the enclosure is maximum where there is stagnation point. Whereas local minima of \( Nu \) is experienced at enclosure corners. As the cylinder moves in upward direction, symmetry of the domain along \( y=0 \) is lost and so the \( Nu \) variation along both cylinder and enclosure wall (figure 3a). Figure 3b shows that, with an increase in \( \delta \) for \( Ra=10^5 \), maximum local Nusselt number is experienced at top surface of the cylinder due to the presence of high thermal gradient at this constricted flow passage. In the presence of rising plume, \( Nu \) decreases gradually to a local minimum value with an increase in \( \theta \) which then subsequently increases again.
3.2. Forced convection through an isothermally heated circular cylinder

Flow past an isothermally heated stationary circular cylinder is investigated in this subsection. A circular cylinder having diameter $d$ is placed in a $30d \times 20d$ computational domain at a distance $10d$ from inlet and bottom of computational domain. The cylinder wall is provided constant hot temperature $T_h$ in comparison to the initially cold uniform temperature at the uniform velocity $U$ inlet. Non-dimensional parameters for the present problem are selected as: Reynolds number $Re=U\infty d/\nu =20$ and Prandtl number $Pr=\nu/\alpha=0.73$. Present solver shows well agreement of variation of coefficient of pressure ($C_P$) with cylinder angle ($\theta$) (figure 4) with He and Doolen et al. [7]. Figure 5 shows the variation of local Nusselt number on the cylinder surface and its comparison with the results obtained by Suzuki et al. [8] and Gan et al. [9] shows excellent match. These results showcase the solver's capability to capture local hydrodynamic and thermal parameters with good accuracy.
Figure 4. Variation of coefficient of pressure ($C_P$) with cylinder angle $\theta$ for $Re=20$. ($\theta$ increases along counter-clockwise direction and $\theta=0$ at stagnation point)

Figure 5. Comparison of local Nusselt number along on the cylinder wall with Suzuki et al. [8] and Gan et al. [9]

3.3. Taylor Couette Flow
In this subsection immersed boundary thermal lattice-Boltzmann (IB-TLB) is applied to Taylor-Couette problem for Dirichlet boundary conditions. Two concentric cylinders of radii $R_1$ and $R_2$ are placed such that $R_2=2R_1$. The inner cylinder is subjected to constant angular velocity $\Omega_p$. The inner cylinder and outer cylinder are provided with constant hot and cold temperature as $T_1=1$ and $T_2=0$ respectively. The non-dimensional parameters for this problem are defined and set as: Reynolds number ($Re=(R_1\Omega_p)(2R_1)/\nu = 50$) and Prandtl number ($Pr=\nu/\alpha =0.73$). In the current simulation, we undergo an order of accuracy test of our solver by varying grid resolution as $\Delta x=1/40$, $1/80$, $1/60$ and $1/320$.

Figure 6. (a) $L_\infty$ and (b) $L_1$ error norm for velocities, pressure and temperature.

Figure 6 shows $L_\infty$ and $L_1$ error norms for velocity, pressure and temperature. It is evident from these figures; errors are degrading monotonically with grid refinement. Moreover, velocity and temperature errors are degrading nominally to first order accuracy with respect to space whereas pressure error is capable of retaining second order accuracy. This degradation of the accuracy as compared to TLBM is due to the discontinuity in the velocity and temperature gradients.
3.4. Forced convection through transversely oscillating heated circular cylinder

In the present section, the solver is checked for its robustness for moving body problem by simulating forced convection through an isothermally heated circular cylinder. As shown in the figure 12, a circular cylinder is placed at location \((X_c,Y_c)=(16d,20d)\) in a domain of size \(40d \times 40d\). The inlet of the domain is provided with cold temperature \(T_c\) uniform velocity inlet \(U\). The uniformly heated cylinder \((T_h)\) is made to transversely oscillate according to \(Y_c(t)=A\sin(2\pi f t)\), where \(A\) is the amplitude of oscillation. The cylinder oscillates for \(Re=200\) with amplitude of oscillation \(A=0.15d\) and frequency of oscillation as \(f=f_e/f_o=0.2\), where \(f_e\) and \(f_o\) are excitation frequency and natural vortex shedding of the cylinder. The Strouhal number for flow past stationary circular cylinder at \(Re=200\) is 0.197 as obtained using our present solver. Figure 8 shows the local Nusselt number over the cylinder wall at \(t=T/2\) (\(T=\)time period of oscillation).

![Figure 7. Schematic for the problem, forced convection through a transversely oscillating heated circular cylinder.](image)

![Figure 8. Comparison of local Nusselt number on the cylinder wall with Zhang et al. [10].](image)

4. Conclusions

In the present paper development of an in-house openMP parallelised immersed boundary thermal lattice Boltzmann (IB-TLB) solver is shown, which is capable of capturing complex thermo-fluidic interaction between fluid and moving structures. The present solver exhibits first-order accuracy in space for velocity and temperature errors whereas pressure error is capable of retaining second-order accuracy for moving boundary problems. Several benchmark problems involving natural and forced convection phenomena for stationary and moving body are presented and the solver exhibits well agreement with existing literature in capturing local parameters. This study creates the base for the solver to simulate several real life applications involving thermal management systems.

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