

Development of a Partially Saturated Cells Based Lattice Boltzmann Solver for Thermo-Fluidic Applications

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in partial fulfillment of the requirements
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by

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“It is not the mountain we conquer but ourselves”

— Sir Edmund Hillary

Dedicated to
Ma and Baba

CERTIFICATE

This is to certify that the work presented in the thesis entitled “**Development of a Partially Saturated Cells Based Lattice Boltzmann Solver for Thermo-Fluidic Applications**” submitted by Sambit Majumder to Indian Institute of Technology Guwahati for the award of the degree of Doctor of Philosophy in Mechanical Engineering is a bona fide record of research work carried out by the student himself under our supervision and have not been submitted elsewhere for any degree or diploma.

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ABSTRACT

This thesis is devoted to the development of a robust and accurate partially saturated cells (PSC) based lattice-Boltzmann (LB) solver for incompressible flows and its application to conjugate heat transfer process. The lattice-Boltzmann (LB) method has emerged as a promising alternative to the conventional Navier-Stokes solvers in the last two decades owing to its simplicity of implementation, utilization of equation of state dismissing any requirement of pressure-velocity coupling, use of Cartesian meshes, and ease of parallelization. Despite certain promising advantages, the conventional treatment of boundary conditions on the curved surfaces using LB approaches suffer staircase representation of the surface. This disparity gets exacerbated in moving boundary problems with continuous interchange of fluid and solid lattice nodes necessitating refilling algorithms at each time, and leads to an increased computational expense. Hence, the need for a fast and robust computational framework for moving body problems has led to the emergence of non-body conformal methods, like the coupled immersed boundary-lattice Boltzmann (IB-LB) method, over the last two decades. Recently, one such variant of the IB-LB method, namely the partially saturated computational cells (PSC) method, has evolved as a promising numerical framework for several moving boundary applications. The key advantage of the technique is that, it employs a unified evolution equation for all media (solid and fluid) present in the computational domain comprising a weighting function based on solid volume fraction and an additional solid collision operator. The latter two elements of the PSC technique are responsible for affecting the boundary conditions to be imposed on the solid body, which may be stationary or moving.

The present thesis demonstrates a comprehensive appraisal of the PSC algorithm subjected to moving boundary scenarios that have hitherto not been explored in open literature but are important for the practical viability of the approach. Key aspects pertaining to the performance assessment of the approach comprise accuracy studies, discrete conservation of properties, dependence of spurious fluctuations on grid resolution for moving boundary problems and Galilean invariance. In addition, the solver's robustness is exhibited for a wide range of non-trivial benchmark problems encompassing stationary and moving boundary problems for hydrodynamic and thermal flows. Furthermore, a novel algorithm for simulating conjugate heat transfer problems using PSC is expounded. A novel strategy for implementation of adiabatic boundary conditions is also elaborated in the present work. Both of these strategies are validated with standard free, forced and mixed convection problems.

Keywords: Partially saturated computational cells, immersed boundary lattice Boltzmann, moving boundary, conjugate heat transfer

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CHAPTER 1

INTRODUCTION

“We repeat that CFD is a growth industry, with an unlimited number of new applications and new ideas just waiting in the future”

- John D. Anderson, Jr., 1995

A general solution of Navier-Stokes (N-S) equations in three-dimensional space and time still remains a dream and is one of the six open Millennium Prize Problems offered by the Clay Mathematics Institute. By the turn of the twentieth century, the necessity to have a more mature form of closed analytical solutions was realized for field problems. Analytical solutions to a large number of problems were not possible, which gave birth to approximate semi-analytical techniques and development of numerical methods. With the advent of high-speed computers and robust numerical algorithms, computational fluid dynamics (CFD) has established itself as capable of churning out much remarkable information for a broad range of practical problems from N-S equations. CFD synergistically complements pure experiments as well as pure theory to deal with the enormous cost and complicated equations respectively, associated with these approaches. The origin of the modern CFD can be traced back to the late 1950s to the T3 group of the Los Alamos National Laboratory under the leadership of Francis H. Harlow. During the 1960s, the pioneering work of Prof. D. B. Spalding and co-workers at Imperial College simultaneously laid the foundation of CFD technology applied to a large number of engineering flows applicable to the industries. With the emergence of several sophisticated algorithms in the past seven decades, it has become feasible to analyze complex flow features pertaining to turbulence, fluid-structure interactions, multiphase flows, micro/nano flows, high-speed

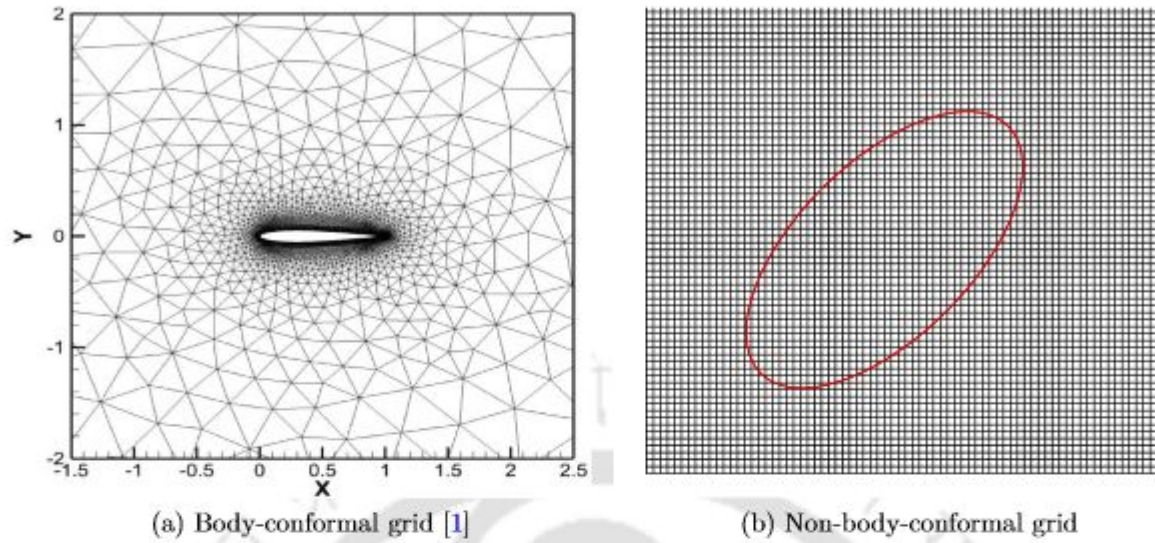


Figure 1.1: Illustrations of body-conformal and non-body-conformal grids.

flows, thermal flows, etc. The core philosophy of such N-S based flow solvers lies in discretizing the governing non-linear partial differential equations into linear algebraic equations. Several discretization techniques like Finite Difference Method (FDM), Finite Volume Method (FVM), Finite Element Method (FEM), Arbitrary-Lagrangian Eulerian (ALE) method, and Lattice Boltzmann Method (LBM), etc., are some of the notable mentions that have evolved immensely since the inception of modern day CFD. These discretized algebraic equations, alongwith appropriate boundary, and initial conditions, are solved over a numerical mesh and iterated until convergence is reached to yield a near-exact solution of the flow field. One of the pivotal requirements towards a consistent and stable solution by any CFD-solver is a good quality mesh of the flow field. Traditionally, body-conformal grids (as shown in Fig. 1.1a¹) were employed across a multi-component flow field. While body-fitted grids can accommodate the accurate implementation of boundary conditions, a major bottleneck occurs when estimating interfacial quantities in a moving boundary problem. In particular, the generation of a body-fitted grid involving complex moving structures and subsequent implementation of the discretized equation requires significant expertise and computational overhead due to the tedious regeneration of conformal meshes in each time step. Furthermore, the estimation of gradients pertaining to the convective and viscous fluxes and resulting spurious fluctuations of the interfacial vector quantities are key challenges of this approach.

¹Reprinted from *Computers and Fluids*, vol. 222, Y.Y. Liu, C. Shu, H.W. Zhang, L.M. Yang and C. Lee, An efficient high-order least square-based finite difference-finite volume method for solution of compressible Navier-Stokes equations on unstructured grids, p. 104926, Copyright (2021), with permission from Elsevier

Therefore, the need for an approach that mitigates the above mentioned issues and simultaneously ensures accurate implementation of the boundary conditions has led to the emergence of non-traditional approaches like mesh-free methods [2] and immersed-boundary (IB) methods [3]. The IB methods have gained prominence over the past decade owing to their inherent requirement of a simple Cartesian grid and thus reducing the dependency on highly skilled users for good quality mesh generation. The true utility of such non-body conformal methods (shown in Fig. 1.1b) also lies in the smooth exchange of information across multi-component interfaces while mitigating the re-meshing process, unlike body-conformal approaches. The IB methods can effectively handle complex bodies and their motion in conjunction with any discretization scheme such as FDM, FVM, FEM, and LBM, etc.

In addition, numerical simulations of fluid flows over complex geometries have been a continuing field of research with efforts to obtain accurate solutions at a lesser computational cost. Anderson [4] has aptly penned, *'Modern CFD is awash with different techniques - some old, some new, some quite simple and straightforward, and some very sophisticated and elaborate'*. The need for fast and robust solvers for three-dimensional problems, particularly involving moving bodies, has led researchers to explore newer techniques and improve existing approaches. Among the several possible techniques that have found favor, the lattice-Boltzmann method has emerged as a promising alternative to conventional finite-volume-based N-S solvers in the last two decades. Key advantages of LBM solvers include simplicity of implementation, utilization of equation of state dismissing any requirement of pressure-velocity coupling, use of Cartesian meshes, and ease of parallelization due to locality of operations. The LBM approach solves the discrete Boltzmann equation [5] at each lattice node for the continuous particle distribution function, which can then be integrated in velocity space to obtain macroscopic variables of interest. Despite these attractive features, implementation issues in the LBM framework must be addressed with care to obtain accurate results. A prominent issue is the need to enforce boundary conditions consistent with the macroscopic flow and this has led to researchers proposing several schemes that include bounce-back [6], interpolated bounce-back [7–9], non-equilibrium extrapolation [10] and non-equilibrium bounce-back [11]. Another drawback with the conventional LBM approach employing a Cartesian lattice is that it approximates curved surfaces using a staircase representation creating a disparity between the physical and simulated boundaries. This disparity gets aggravated in moving boundary problems with continuous change of fluid and solid lattice nodes necessitating reconstruction of distribution functions at each time, which leads to an increased computational expense.

Researchers have therefore devised methodologies that blend the LBM approach with the IB philosophy. The key idea is to represent the body that is considered "immersed" in the lattice by means of a set of Lagrangian surface points while the macroscopic variables are determined at the Eulerian lattice nodes. After solving the governing equations, the information available in the Eulerian nodes (such as velocity, pressure, and temperature) are interpolated to the Lagrangian boundary points using a suitable spreading function. These are then employed to evaluate the forces due to particle motion and fluid-particle interactions at the Lagrangian points, and these forces are then interpolated back to the lattice nodes. This two-way exchange allows coupling between the solid and fluid by effectively communicating the presence of bodies to the underlying lattice while also ensuring that fluid-solid interactions are accurately computed.

Thus, the present thesis is devoted towards the development of a general in-house immersed-boundary lattice-Boltzmann (IB-LB) solver. To achieve this overall goal, the author begins by carrying out a comprehensive literature survey of existing numerical efforts in developing an IB-LB computational framework for thermo-hydraulic flows.

1.1 Development of lattice-Boltzmann method

The lattice Boltzmann method has its historical provenance in Lattice Gas Automata (LGA) [12, 13], which conceptualizes the discrete particle-based proposition, thereby presaging the physical system as a unification of multiple fictive particles with constrained motion. The nature of migration of such particles to their respective neighborhoods is governed by local collision, translation, and reaction rules, consequently facilitating the replication of most of the macroscale fluid behavior. The boolean interactions allow near-perfect imitation of collision while being numerically stable and expediting the easier implementation of boundary conditions, along with the promise of aiding massive parallelization. However, the same boolean redistribution rule invariably insinuates substantial statistical noise, even with lattice in equilibrium, necessitating spatial and/or temporal averaging for smoothed macroscopic profiles. LGA faces further challenges from the intrusion of anisotropy in the Navier-Stokes equation, possible non-Galilean invariance, and velocity-dependent pressure. In an effort to surmount such impediments, with the primary compulsion being the eradication of statistical noise, McNamara and Zanetti [14] proposed the lattice-Boltzmann equation (LBE) that replaces the boolean particle occupation variable with its anticipated value retrieved from the mesoscopic kinetic theory, thereby stimulating the evolution of the flow field on timescales comparable with mean collision time. Later Higuera

and Jiménez [15] proposed a linear collision operator to reduce computational cost and excessive memory requirement associated with the non-linear LBE. Although the utilization of the equilibrium distribution function in collision operator originated from the LGA, the limitations associated with the velocity-dependent pressure and density-dependent convection coefficient due to lack of Galilean invariance persisted. Eventually, these issues were eliminated by invoking Maxwell-type equilibrium distribution functions [16, 17]. This simplified version of collision operator was originally proposed by Bhatnagar, Gross and Krook [18] is also popularly known as BGK collision operator. It utilizes a constant value for the relaxation time (τ) and has the capability to conserve mass, momentum, and energy while recovering the accurate behavior of the macroscopic N-S equations.

The LBM has established itself as a robust numerical framework that can capture discontinuous mechanics and hydrodynamics (Knudsen number less than unity), as well as its kinetic nature can accurately predict the discontinuous phenomena involving Knudsen number close to unity without using large computational resources. Presently, it has been widely used in various field of research like multiphase flows [19, 20], non-Newtonian flows [21], heat transfer [22, 23], porous media [24, 25], turbulent flows [26, 27] and microfluidics [28, 29], to cite a few. Some salient features of the LBM in comparison to the conventional N-S based solvers are enlisted as follows-

- The fundamental governing equations pertaining to LBM are at mesoscopic level compared to the macroscopic transport equations used in the traditional CFD solvers, like the continuity, the N-S equations for momentum, and the energy equation.
- The advection term of LBE is linear in contrast to the non-linear operator in N-S equations.
- Pressure is evaluated using the equation of state in LBM that facilitates a scope for efficient parallelization while relying on the pressure-Poisson equation in N-S solvers is a tedious and expensive affair.
- In LBM, the Boltzmann transport equation is discretized in a lattice space, velocity, and time to yield the discretized LBE. This evolution equation tracks the particle distribution function (*pdf*) and recovers the macroscopic parameters like velocity, pressure, and temperature through velocity moments of these *pdf*s. The recovery of macroscopic N-S equations from the discretized LBE can be achieved through the Chapman-Enskog multiscale expansion. While in conventional CFD solvers, the N-S equations are discretized into linear algebraic

equations in macroscopic time and space using a suitable discretization technique. These system of equations, along with initial and boundary conditions, are iterated until convergence to yield macroscopic variables like velocity, pressure, and temperature.

- If the functional form of the collision operator is known *a priori*, the algebraic operations pertaining to the discretized LBE are explicit in nature and local to the lattice nodes. It facilitates highly parallelizable schemes in LBM in comparison to the N-S solvers.

Despite possessing several advantages over traditional CFD approaches, LBM suffers from serious challenges in implementing boundary conditions due to its kinetic nature. The boundary conditions are mostly prescribed in macroscopic quantities; however, a standard realizable counterpart at the mesoscopic level is challenging. For instance, a no-slip boundary condition on a solid surface can be directly implemented by taking zero relative velocity of the tangential component of the velocity field in N-S based solvers. Whereas, in LBM, due to its kinetic nature, the particle density leaving out a system must be replaced by particle density entering it. The properties of these incoming particles set the basis for the lattice-Boltzmann (LB) level boundary conditions, and they can be either known *a priori* or computed from the information available through the leaving particles. Generally, a perfect knowledge of the properties of these particles is not available, and some approximations are used to formulate the boundary conditions. The fundamental difficulty associated with the LB boundary condition is that the particles' mesoscopic level degree of freedom is more than the macroscopic moments that they need to satisfy. Conventionally, the bounce-back (as depicted in Fig. 1.2) or multireflection schemes [30, 31] were used to treat the no-slip boundary condition. Despite being old, it is still a popular method to treat a wall boundary in the LB community due to its simplicity of implementation. Zou and He [11] further proposed specified pressure and velocity conditions in terms of non-equilibrium distribution function for LB boundary conditions that maintain second-order spatial accuracy. Chen et al. [32] proposed an extrapolation scheme to deal with open boundaries by taking a fictitious layer of nodes outside boundaries. Accurate implementation of boundary conditions is already arduous, and the complexity increases further for fluid systems involving moving and complex boundaries. To attempt such problems, Fillippova and Hänel [7], Mei et al. [8], Bouzidi et al. [9], Yu et al. [33] proposed bounce-back like schemes to appraise unknown *pdfs* at curved boundaries based on the fraction of intersected link crossing the interface in fluid region. These schemes were second-order accurate but simultaneously encountered several challenges. Some notable limitations pertaining to these schemes are

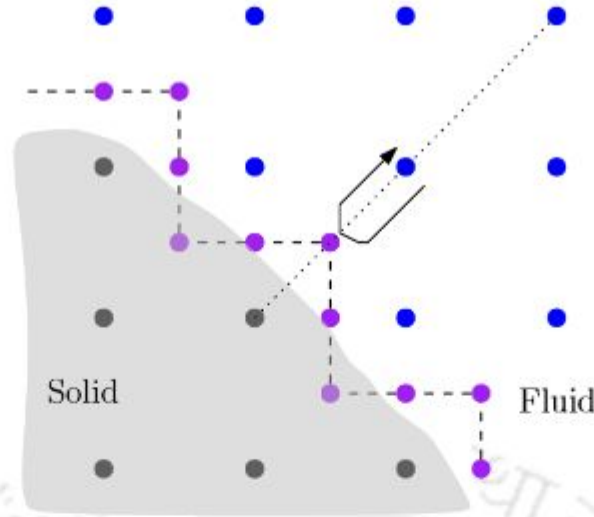


Figure 1.2: Illustration of a basic curved wall treatment scheme. Blue and grey circles represent fluid and solid lattice nodes, respectively. The purple circles denote the half-way locations intended for the bounce-back of distribution functions in half-way bounce-back schemes. The dashed line represents a staircase like approximation of the curved surface.

presented below-

- Schemes are unable to predict the accurate representation of the solid-fluid interface due to staircase-like approximation (as shown in Fig. 1.2) of the boundaries.
- The continuous movement of the solid body inside the computational domain results in birth and death of the solid-fluid node as shown in Fig. 1.3. This further necessitates ancillary treatment using refill algorithms [34, 35] to determine the unknown distribution functions and conserve mass and momentum simultaneously. Such treatments increase the computational time and complexity of the algorithm.
- The schemes yield spurious fluctuations in the hydrodynamic force calculation [34, 36] (Fig. 1.4)². Furthermore, interpolations associated with these schemes greatly affect the mass and momentum conservation at the boundary.
- Refinement of lattice mesh becomes necessary for capturing high velocity and thermal gradient zones. Multiblock techniques [37] used to account for this issue are computationally expensive and possess complex implementation.

The need for a fast and robust computational framework for moving body problems encountered in fluid-structure interaction has led to the emergence of the coupled

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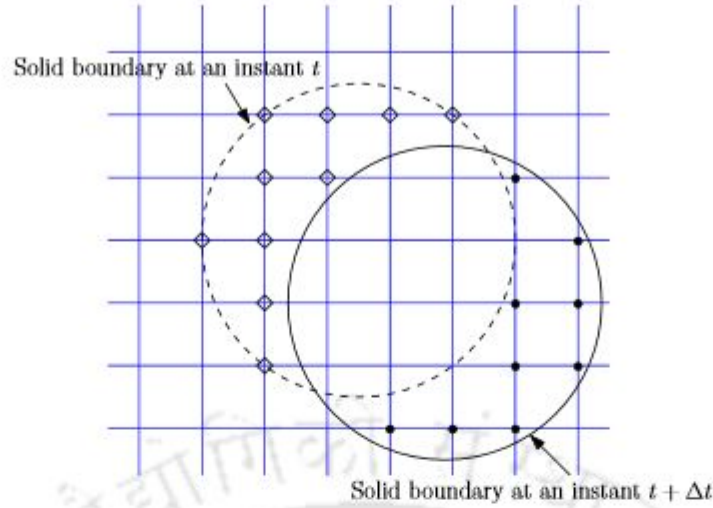


Figure 1.3: Birth-and-death of cell identity during moving boundary problem. The circular and diamond symbols demonstrate the birth and death of solid lattice nodes at an interval Δt .

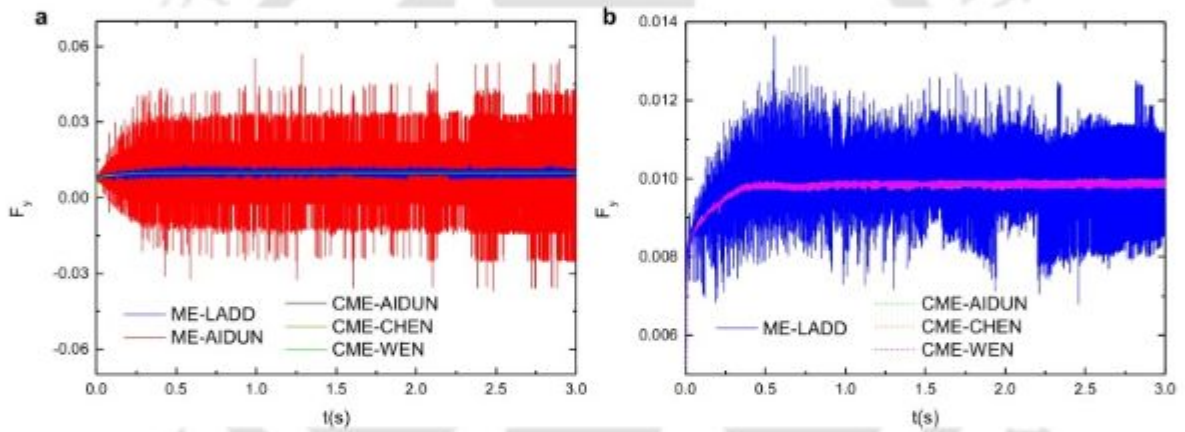


Figure 1.4: Time history of spurious force fluctuations yielded by bounce-back like schemes [36].

immersed boundary method over the last two decades. Specifically, the inherent requirement of uniform Cartesian mesh in both IB and LB methodologies has led to their amalgamation. Among several immersed boundary–lattice Boltzmann methodologies (IB-LB) available in the open literature, we will now briefly review some of the prominent variants in the next section.

1.2 Immersed boundary-lattice Boltzmann (IB-LB) Methods

The term '*immersed boundary method*' was first coined in the pioneering work of Peskin [38], which demonstrates the numerical simulation of blood flow associated with

cardiac mechanics. The key idea of the method is to employ a non-body conformal grid with the complex boundary represented by a set of Lagrangian points while immersed into an Eulerian fluid domain. Upon solving the governing equations on Eulerian nodes, various flow field parameters such as velocity, pressure, and temperature are spread to Lagrangian boundary nodes. The resulting force that evolves out of particle motion and fluid–particle interactions at Lagrangian nodes can now be distributed into Eulerian fluid nodes while simultaneously advecting the Lagrangian nodes to account for the motion of the body. A detailed utility of the IB philosophy can be found in the review work of Mittal and Iaccarino [3].

Among the earliest notable efforts to develop the IB-LB framework was the penalty-force approach proposed by Feng and Michaelides [39] in a Lagrangian–Eulerian framework which considers deformable particles with a high stiffness coefficient and adds to the evolution equation an external force density term that accounts for fluid and particle velocity field. This approach was used to study a couple of fluid–particle interaction problems—DKT motion of two particles and sedimentation of multiple particles, from which the authors concluded that coupled IB-LB method is capable of accurately resolving fluid–particle boundary condition. They also found that the method is more accurate than bounce-back schemes and reduces initial fluctuations in particle forces and torques, which are common in general LB approaches. The penalty-force approach, however, suffers the limitation that it requires a careful choice of user-defined free parameters. This limitation was overcome in the direct forcing immersed boundary-lattice Boltzmann (DF-IB-LB) [40] method by adding a forcing term in momentum equation that enforces no-slip condition on the boundary and was found to be efficient in simulations of high Reynolds number flows. Their work high-

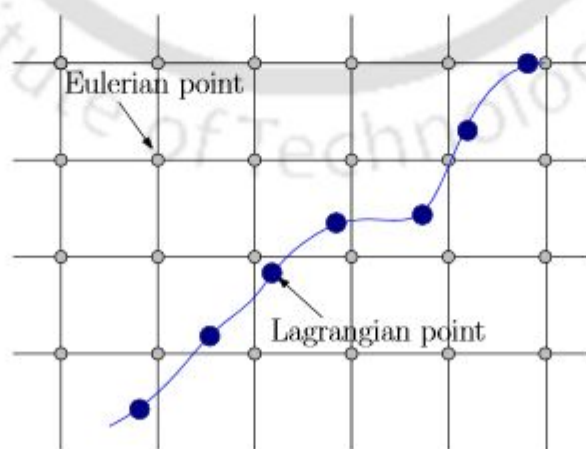


Figure 1.5: Illustration of the Immersed Boundary method. The Lagrangian points represent the boundary, and the intersection of the mesh lines represents the Eulerian fluid points.

lighted the capability of the approach to offer a smooth computational boundary as compared to the conventional "bounce-back" schemes used in LBM. While they remarked that the DF-IB-LB method possesses the same order of accuracy as the LB method, no quantitative data were provided to support this claim. Dupuis et al. [41] introduced the interpolating forcing approach that exhibited an order of accuracy of 1.9 in drag coefficients of an impulsively started cylinder as compared to a 1.5 convergence rate using direct-forcing method. Although the interpolating forcing approach is a nearly second order accurate method, it involves tedious interpolations, which in turn increases the computational cost and time for moving boundary problems.

Yet another approach is the momentum exchange based method of Niu et al. [42], where the particle distribution function on the boundary is obtained from interpolation using Lagrangian polynomials from the Eulerian lattice, but is relatively more difficult to implement compared to other approaches. Wu and Shu [43] devised the velocity correction based IB-LB approach where the velocity is contributed in two parts, one from density distribution function referred to as intermediate velocity and the other from the external forcing term considered as velocity correction. These velocity corrections are calculated so that non-slip boundary conditions are imposed on the solid boundaries. Zhang and co-workers [44] formulated an iterative force correction method to obtain external force term involved in the LB equation that can accurately implement no-slip boundary conditions on solid boundaries considering the effects of present and next time steps. They employed Lagrangian polynomial interpolations instead of the Dirac delta function to determine velocities on boundaries from neighboring fluid nodes.

An interesting approach proposed by Noble and Torczynski in the late nineties is the partially saturated computational cells method (PSC) [45]. This method may also be classified as belonging to the IB-LB class of schemes, although it has not been traditionally referred to in that manner. This technique employs a unified evolution equation for all media (solid and fluid) present in the computational domain with a weighting function based on solid volume fraction and an additional solid collision operator. The latter two elements of the PSC technique are responsible for effecting the boundary conditions to be imposed on the solid body which may be stationary or moving. Studies carried out for flow past a stack of cylinders showed the approach to be second-order accurate and capable of accurately computing the flow past multiple objects. Strack et al. [46] carried out several test cases of stationary and moving spheres in creeping flow regime using PSC. Their studies showed that velocity, force and torque errors exhibited a second-order decay with grid refinement for stationary

body problems while the force and torque errors demonstrated quadratic and linear decay in a settling sphere problem. Chen et al. [47] reported that the sudden transformation of fluid nodes into solid nodes in moving boundary problems leads to a violation of geometric conservation laws (GCL) that were responsible for spurious force oscillations (SFOs). To mitigate these oscillations, they coupled the ghost-fluid method along with the cut-cell based PSC methodology to treat the solid boundary in sharp-interface IB sense enforcing the GCL.

Owen et al. [48] proposed a coupled PSC-DEM framework for solid-fluid interaction problems where the bounce-back variant of solid collision operator was found to be more accurate than other variants. However, they found that the method failed to compute the shear stresses accurately in the low Reynolds number regime. A more recent effort by Najuch and Sun [49] has analysed the role of the solid collision operator in two variants of the PSC method in computing the hydrodynamic stresslet and hence rheology of granular suspensions. Rettinger and Rde [50] have carried out resolution and viscosity dependence studies of several variants of momentum exchange method (MEM) and PSC in a periodic array of spheres in Stokes flow regime. They found that using the superposition model of solid collision operator led to less than second order convergence, whereas the bounce back and Holdych's model resulted in second order convergence rate with grid refinement. Interestingly, the MEM variants, despite having non-smooth convergence of errors, exhibited smaller errors than the PSC approach. Their studies also highlighted that while MEM variants yielded force errors independent of choice of relaxation time (τ), force errors from PSC variants exhibited strong dependency on τ . The authors also studied these variants in purview of fluid-solid interaction of a moving sphere in ambient fluid in different flow regimes and concluded that, while MEM approaches could provide an accurate prediction of stream-wise velocities, the span-wise velocities were accurately predicted when PSC techniques was employed.

A more recent study on the PSC approach and its variants vis-a-vis moving boundary methods (MBM) was performed by Haussmann and co-workers [51] with an emphasis on Galilean invariance, volume approximation methods and refill algorithms. The volume approximation methods in PSC approach were found to possess smaller Galilean invariance errors as compared to refill algorithms used for MBMs, along with the smaller pressure fluctuations and better momentum conservation, which were attributed to the continuous description of the domain due to diffusive nature of the algorithm. They also extensively investigated the problem of vortex-induced vibrations of a cylinder at $Re=100$ and identified the best algorithms in the class of PSC and

MBM approaches. It is also important to note herein that both the studies of Rettinger and R  de [50] as well as those of Haussmann et al. [51] have reported a lower order of spatial accuracy (close to unity) for the PSC approaches as compared to the MBM frameworks. In recent times, the PSC approaches have been extensively employed in the field of computational rheology, such as to study particle migration and deposition characteristics in a microchannel [52] and particle suspension characteristics exposed to thermal effects involving conjugate heat transfer and temperature-dependent viscosity [53]. They have also been applied to investigate large-scale geophysical flows involving dynamics of densely packed granular flows and pore-scale physics [54], suffusion process in granular flows [55], seepage failure of saturated granular soils [56] and interaction between complex shaped air borne particles with porous media structures in filtration processes [57] among other studies in porous media and rheological flows [49, 58–60].

1.3 Immersed boundary-thermal lattice Boltzmann (IB-TLB) Methods

The previous section illustrated that the direct-forcing-based IB-LB method has been extensively used in hydrodynamic and isothermal problems. Likewise, the direct-forcing thermal IB-LB method also paved its way as an efficient methodology that can incorporate thermal boundary conditions accurately. The forcing term principles in both momentum and energy equations are same; the difference lies in the fact that only Dirichlet type boundary condition is considered in momentum-forcing while both Dirichlet and Neumann types can be considered in energy-forcing immersed boundary method. Zhang et al. [61] presented a direct-forcing immersed boundary scheme over the underlying predictor-corrector-based finite-difference framework. The proposed scheme offers an independent selection of the number of IB grid points irrespective of the resolution of the computational grid and also ensures the implementation of boundary conditions on IB locations intersecting the grid points as well as in any locations between these grid points. The methodology revealed second-order accurate spatial convergence for Dirichlet and Neumann-type boundary conditions. It also produced fewer spurious kinks and a smoother curve compared to the existing literature during the estimation of the local Nusselt number for heat convection over a circular cylinder in stationary and imposed motion scenarios. Jeong et al. [62] proposed a coupled immersed boundary thermal lattice Boltzmann method based on the equilibrium internal energy density approach. The external forcing term is constituted using the "equilibrium velocity" that takes care of the change of momentum as proposed by

Shan and Chen [19]. The increase in error norms with the increase in relaxation time for the energy model was attributed to noticeable artificial boundary slip and artificial boundary temperature. The algorithm is tested over natural convection phenomena involving heated square and circular cylinders inside a cold wall square enclosure, which revealed that the results are in good agreement with the previous literature. However, the algorithm still possesses an arbitrariness in the selection of free parameters and hence prone to induce instabilities.

Kang and Hassan [63] developed a direct-forcing based immersed boundary thermal lattice Boltzmann model based on two thermal LB models, *viz.*, double population model and a hybrid model with advection-diffusion equation. In contrast to the use of Dirac-delta function in hydrodynamic direct forcing diffuse interface IB-LB method [40], they incorporated a sharp-interface-based interpolation scheme. The hybrid thermal LB (TLB) model consumed 50% less computational time as compared to the simplified thermal LBE model. However, comparable error norms in Nusselt estimation were reported by them. Khazaeli et al. [64] proposed ghost fluid-based TLB method using a double population based model. The ghost fluid method decomposes the unknown distribution function of ghost nodes at solid-fluid interface into its equilibrium and non-equilibrium parts. The equilibrium part is reconstructed using the extrapolated quantities (e.g., velocity, density, distribution functions, etc.) from the corresponding image points, while the non-equilibrium parts are evaluated using bounce-back schemes. The method exhibited second-order spatial order of accuracy and good agreement with previous literature when tested upon cylindrical thermal Couette flow, natural convection in an annulus, and convective heat transfer in a semi-circular lid-driven cavity problem. Seta [65] proposed a redefined temperature source term for implicit correction immersed boundary thermal lattice Boltzmann method, which enhances the accuracy of the boundary conditions for temperature and velocity as well as restricts penetration of streamline across the immersed body. The method revealed that the boundary errors strongly depend on the choice of relaxation time. The value of relaxation time less than unity was recommended to ensure accuracy and simultaneously reduce boundary slip for temperature.

Hu et al. [66] proposed a diffuse-interface immersed-boundary thermal lattice Boltzmann method for Dirichlet, Neumann, and Robin type thermal boundary conditions. The Dirichlet type temperature boundary condition is realized using an iterative procedure. Neumann and Robin type boundary conditions are implemented through derived jump conditions of derivative of temperature and further smoothening them using the Dirac-delta function. Subsequently, implicit heat flux equations are

evaluated on the immersed Lagrangian nodes, and the temperature field is corrected by spreading the heat flux to neighboring Eulerian nodes. The algorithm exhibited second-order spatial accuracy in maximum and L_2 velocity errors when tested upon the Taylor-Green vortices problem with an embedded stationary cylinder. When tested upon a rotational problem, the algorithm exhibited first-order spatial accuracy for both temperature and velocity error norms for all types of boundary conditions. This degradation of the order of accuracy was attributed to the lack of smooth transition of velocity and temperature field at the solid-fluid interface, unlike the previous test case.

Eshghinejadfard and Thévenin [67] presented the efficacy of the direct forcing and direct heating IB-TLB method for two and three-dimensional flow simulations involving natural convection heat transfer phenomena in stationary and moving bodies. Direct-forcing IB-LB method suffers a limitation of momentum leakage across the solid surface and subsequently leads to boundary velocity slip and temperature jump at the solid-fluid interface. To mitigate this drawback, a multi-direct-heating scheme [68] is proposed that applies the direct-forcing and direct-heating in momentum and thermal governing equations, respectively, until the no-slip condition is satisfied. Wu et al. [69] proposed an iterative correction IB-TLB method that modifies the heat source term as in Cheng's approach [70] for hydrodynamic IB-LB. The proposed scheme can eliminate the temperature jump irrespective of the choice of relaxation time. However, the spatial order of accuracy for temperature errors are found to be first order, and the use of the first-order Dirac delta function is attributed to its cause. Seta et al. [71] undertook an extensive numerical and analytical analysis of two different types of iterative correction method *viz.*, Guo's forcing [72] and Cheng's split-forcing [70] approaches to demonstrate boundary velocity slip and temperature jump in IB-TLBM with a two-relaxation-time (TRT) collision operator. The proposed iterative correction method and multi-direct forcing method alongwith TRT collision model can eliminate velocity slip and temperature jump even at high relaxation times, unlike the commonly used SRT multi-direct forcing methods. However, all IB-TLBM models analyzed by Seta et al. [71] exhibited first-order convergence rate in velocity, temperature, and torque errors with respect to grid refinement, whereas a superlinear convergence is observed in pressure.

Suzuki et al. [73] proposed a multi-direct heating IB-TLB method that ensures implementation of Dirichlet type boundary condition for the temperature field by undergoing an iterative correction process of heat source term while the Neumann type temperature field is determined from the difference between desired heat flux and the temporary temperature field regardless of the boundary. This method, too exhibited

first-order convergence in temperature and rate of heat errors with respect to grid refinement for both types of boundary conditions. The degradation of the order of accuracy while coupling IBM with LBM, unlike the second-order accurate LBM, was attributed to the discontinuous temperature gradient at the solid-fluid interface. Apart from validating the algorithm with several stationary and moving boundary heat transfer benchmark problems, the authors also reported to consider a virtual boundary in order to accommodate the effective thickness of immersed boundary. Moreover, the incorporation of internal heat effect for moving boundary problems subjected to iso-heat flux conditions was highlighted by them. However, the internal heat effect can be neglected for problems having iso-thermal conditions with constant temperature unless subjected to space-and/or time-dependent temperature.

Kefayati [74] proposed an IB-LB method to simulate different thermal and thermosolutal problems using Newtonian and non-Newtonian fluids. The method can also implement Dirichlet and Neumann boundary conditions straightforwardly by macroscopic parameters, unlike the complex conventional approach of converting them to distribution functions at the LB level. In contrast to the previously established direct heating IB-TLB methods that possess expensive computational steps to treat temperature gradient, Wang et al. [75] proposed a novel way of expressing discrete heat source terms at the mesoscopic level. The method reduces computational complexities to treat Dirichlet and Neumann boundary conditions without incorporating any artificial parameters. Nevertheless, the method exhibited first-order accurate spatial convergence for Dirichlet and Neumann-type boundary conditions. Chen et al. [76] proposed an immersed boundary-simplified thermal lattice Boltzmann method constituting predictor-corrector steps in order to facilitate the boundary conditions. The predictor step evaluates the intermediate flow field regardless of the immersed boundary. The corrector step rectifies the flow variables by incorporating the boundary-condition enforced IBM as a source term in the evolution equation. Although the method ensures the least use of virtual memory and eliminates the penetration of streamlines or isotherms over the solid wall, but experiences a bulky computational sequence. Romanus et al. [77] proposed a domain transferring scheme to enable the simulation of non-spherical particle in an infinite domain. However, the scheme reduced the memory demand but exhibited a first-order spatial order of accuracy in velocity errors. Suzuki et al. [78] used the extended version of their 2D model of ice slurry flow to investigate the cooling performance of three-dimensional ice slurry flow in a square duct using the thermal IB-LB method.

To mitigate the scalar mass conservation issue pertaining to the grid-based meth-

ods in moving boundary problems, Zhang et al. [79] coupled the Random Walk Method (RWM) and PSC-based Discrete Element Method (DEM). The proposed scheme utilized the RWM to evaluate scalar transport equations and DEM to handle the complex fluid-particle interfacial dynamics and thus strictly satisfies the scalar mass conservation. Chen and Müller [80] introduced the partially saturated computational cells method for thermal problems. The asymptotic analysis of the method while considering the Dirichlet type boundary condition indicated it to be a second-order accurate method. Furthermore, the numerical analysis of the method for a pure heat conduction problem confirmed second-order spatial convergence in Nusselt number and temperature errors. The authors also presented the method's efficacy in accurately estimating heat transfer characteristics of static and moving boundary problems. The original PSC algorithm [45] for hydrodynamic boundary conditions possesses the promising potential to solve incompressible fluid flows past complex moving structures with lesser spurious force oscillations. It can efficiently diffuse the solid-fluid interface present in a non-body-conformal grid while accurately satisfying the boundary conditions. These factors motivate us to further investigate the methodology for heat transfer problems.

1.4 Objectives of the thesis

In light of the comprehensive literature review carried out in the previous section, one may conclude that the PSC framework has not been the subject of a thorough analysis for classical hydrodynamic and heat transfer problems, unlike its IB counterparts in the finite volume framework [81–84]. In particular, hydrodynamic studies concerning the discrete conservation, accuracy on stationary and moving body problems, and dependence of spurious force oscillations with lattice size have not been discussed in detail in the open literature to date. Moreover, investigations using PSC methodology for heat transfer problems are very limited, even though it possesses appealing potential to simulate incompressible flows. So far, Chen and Müller [80] presented the PSC algorithm for conduction-dominated flow and mostly forced convection problems. Present work's emphasis will be largely devoted to benchmarking the PSC methodology over a broad spectrum of heat transfer problems encompassing forced, natural, and mixed convection phenomena while the particle is subjected to stationary, imposed, and induced motion scenarios.

Furthermore, the PSC method identifies itself as an immersed boundary method; however, it differs from the conventional IB-LB approaches as it offers a unified evolution equation for all the media in a physical system. A comparative analysis of the

PSC and DF-IB-LB method is also presented for incompressible hydrodynamic and thermal flows to review the viability of the PSC philosophy at par with the direct-forcing philosophy. The extensive literature survey also unveiled that there exists no work which utilizes the PSC methodology for practical scenarios involving conjugate heat transfer. Thus, the author has extended his experience and understanding to develop a novel PSC strategy for simulating conjugate heat transfer problems. It has further motivated the author to utilize this philosophy to employ an adiabatic boundary condition to an immersed surface. It must be mentioned here that the PSC methodology investigated in this thesis expects constant values of velocity and temperature at a lattice node, with no provision to accommodate their gradients. Thus it becomes challenging to implement the Neumann boundary conditions, particularly with this class of diffuse interface IB methods. The present thesis's focal points of investigation using the PSC framework may be summarized as follows-

1. Development of a robust partially saturated computational cells (PSC) solver for incompressible flows with stationary and moving bodies:

- Studies of spatial accuracy and conservation properties.
- Spurious force oscillations in moving body problems and role of lattice resolution.
- Effect of virtual (added) mass on accuracy of hydrodynamic force and torque coefficients.
- Numerical simulations and benchmarking of incompressible hydrodynamic flows involving single and multiple bodies with imposed as well as induced motion.

2. Development of the PSC solver for thermal flows involving stationary and moving bodies:

- Investigation of spatial order of accuracy and Galilean invariance of PSC framework for thermal flows.
- Detailed analysis of PSC evolution equation to recover the macroscopic energy equation using Chapman-Enskog multiscale analysis.
- Development of a mechanism for evaluating the local temperature gradients over the immersed surface and verify its congruity in the subsequent simulations.
- Numerical benchmarking of the PSC framework for a wide range of thermal flows encompassing natural, forced and mixed convection flows along with stationary, imposed, and induced motion of the immersed particle.

3. Comparative analysis of the PSC solver with respect to the direct-forcing IB-LB methodology:

A comparative study of the aforementioned methodologies in terms of spatial order of accuracy, discrete conservation of the properties, Galilean invariance, and quantification of the effect of lattice size in spurious force oscillations is presented. The study endorses the PSC algorithm's applicability for thermo-fluidic applications comparable with the popular DF-IB-LB methodology.

4. Development of a novel PSC algorithm to simulate conjugate heat transfer problem:

The development of a novel algorithm to simulate conjugate heat transfer problems using the PSC strategy and benchmarking the solver across natural, forced, and mixed convection flows is demonstrated. It further exhibits a novel strategy to implement adiabatic boundary conditions at immersed surfaces. The strategy is validated through benchmarking pure conduction, natural and mixed convection cases.

It must be reiterated that such a full-fledged assessment of the PSC approach has not been forthcoming in literature to the best of the author's knowledge and is clearly a novel contribution to the field which can be beneficial to computational LB community. The solver used for the numerical simulations in the present thesis is developed in-house using openMP shared memory parallelization and utilizes the computational facilities available at the Indian Institute of Technology, Guwahati, India.

1.5 Outline of the thesis

The remainder of the thesis is organized as follows. Chapter 2 demonstrates a brief overview of the governing equations of the LBM and the mathematical formulation of the PSC approach with a discussion of the computation of solid volume fraction, hydrodynamic forces, and local temperature gradients. Chapter 3 presents a study of the PSC approach's accuracy and quantification of the mass defect and SFOs pertaining to incompressible viscous flows. A wide range of test problems that involve stationary and moving bodies, including fluid-structure interaction, are carefully examined in this chapter. The subsequent chapter 4 highlights the accuracy and Galilean invariance of the method for thermal flows. Furthermore, the method is investigated in a broad spectrum of benchmark test cases, which include natural, forced, and mixed convection phenomena along with stationary, imposed, and induced motion of the particle. This is followed by chapter 5, wherein a comparative analysis of the PSC and DF-IB-LB approaches exhibit their efficacies and robustness for simulating thermo-hydraulic

problems. Chapter 6 details the development of the PSC algorithm for conjugate heat transfer problems and a novel strategy for implementing adiabatic boundary conditions on the immersed surface. Finally, chapter 7 showcases the salient conclusions from the extensive investigations and provides directions for future efforts with this approach.



CHAPTER 2

GOVERNING EQUATIONS AND MATHEMATICAL PRELIMINARIES

“No knowledge can be certain, if it is not based upon mathematics or upon some other knowledge which is itself based upon the mathematical sciences”

- Leonardo da Vinci, 1425-1519

The chapter demonstrates a brief overview of the governing equations of the lattice Boltzmann method applicable to the incompressible hydrodynamic and thermal flows. Subsequently the partially saturated computational cells method is introduced for the conservation equations of momentum and energy. The strategy for evaluation of solid volume fraction, interacting forces and local Nusselt number over the curved surfaces is presented meticulously.

2.1 Basic LBM formulation

The lattice-Boltzmann method (LBM) has originated from Lattice Gas Automata (LGA) [12, 13], which utilizes discrete population-based formulation to describe a physical system. The fluid motion in lattice gas is dictated by local collision, translation, and reaction rules which can come across many microscopic level complex fluid behaviors. LGA method utilizes boolean/discrete distribution rules that specify the

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presence or absence of populations at any node. Over the years, LBM emanated with the intention to replace boolean particle occupation variables with continuous particle distribution function in the Lattice Boltzmann equation. Particle distribution functions evolved from the kinetic theory of gases, which signifies the probable density of a particle being found at a particular location and instant. Discretized lattice Boltzmann equation can be evaluated at each lattice node to obtain particle density using collision and relaxation rules and then propagate (stream) them to the neighboring nodes. Integration of these distribution functions in velocity space yields macroscopic variables such as density, velocity, and temperature. Thus, the LB method can capture discontinuous mechanics and hydrodynamics (Knudsen number less than unity), as well as its kinetic nature, offers to predict discontinuous phenomena involving Knudsen number close to unity regardless of using large computational resources. Numerical simulation using LBM possesses less computational effort, easy algorithm, and can be naturally adapted to parallel computing. LBM also offers explicit first order linear partial differential equation of hyperbolic nature, which utilizes equation of state dismissing any requirement of pressure-velocity coupling.

The translation of particles within lattice is realized in LBM in terms of the particle distribution function $f(\mathbf{x}, \boldsymbol{\zeta}, t)$, envisaged as the probability of finding a particle at a specific location at an instant. While the analytical solution of the Boltzmann equation itself is too cumbersome, with the primary variable being a function of five variables in a simple 2D lattice, its numerical form discretized in velocity space is rather simple to implement. The discrete form of the force-free Boltzmann equation yields a simple hyperbolic shape, where the exodus of the distribution function $f_i(\mathbf{x}, t)$ with velocity $\mathbf{c}_i$ in the i^{th} vectorial direction is presented as,

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i^{BGK}(\mathbf{x}, t) \quad (2.1)$$

where, Ω_i^{BGK} is the collision operator proposed by Bhatnagar, Gross and Krook [18], which relaxes the population towards the equilibrium distribution (f_i^{eq}) based on the relaxation time (τ_f) as,

$$\Omega_i^{BGK}(\mathbf{x}, t) = \frac{\Delta t}{\tau_f} [f_i^{eq}(\rho_f, \mathbf{u}) - f_i(\mathbf{x}, t)] \quad (2.2)$$

Embracing a functional form of f_i^{eq} is an important step towards recovering the Navier-Stokes equation. Many plausible variations are available in literature based on the selected set of conservation equations and derived from multi-scale Chapman-Enskog expansion. A well-established formulation, primarily favored for incompressible flows

owing to its simplicity, robustness and linearity, in a nine-speed square lattice (D2Q9i) is adopted here, and the same is presented below.

$$f_i^{eq}(\rho_f, \mathbf{u}) = w_i \left[\rho_f + \rho_0 \left\{ \frac{\mathbf{u} \cdot \mathbf{c}_i}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{c}_i)^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} \right\} \right] \quad (2.3)$$

Here c_s is the acoustic speed ($= \mathbf{c}/\sqrt{3}$), $\mathbf{c}$ is the lattice velocity ($= \Delta x/\Delta t$), and Δx and Δt are representatives of the adopted grid spacing and time step respectively. The fluid density (ρ_f) can be expressed as $\rho_f = \rho_0 + \delta\rho_f$, with ρ_0 , $\delta\rho_f$ and $\mathbf{u}$ respectively being fluid density averaged over the entire domain, density fluctuation localized to a cell and nodal fluid velocity. A fully complete set of information regarding the selection of weight w_i germane to the concerned velocity direction $\mathbf{c}_i$ in a D2Q9i lattice arrangement is summarized in Fig. 2.1. Macroscopic quantities such as density and velocity can be recovered by taking velocity moments of the distribution function as,

$$\rho_f(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t) \quad (2.4a)$$

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho_0} \sum_i f_i(\mathbf{x}, t) \mathbf{c}_i \quad (2.4b)$$

while the physical properties of the concerned fluid can be introduced through the relaxation time as,

$$\nu_f = \left(\tau_f - \frac{\Delta t}{2} \right) c_s^2 \quad (2.5)$$

The pressure in LBM simulations can be straightforwardly obtained using the equation

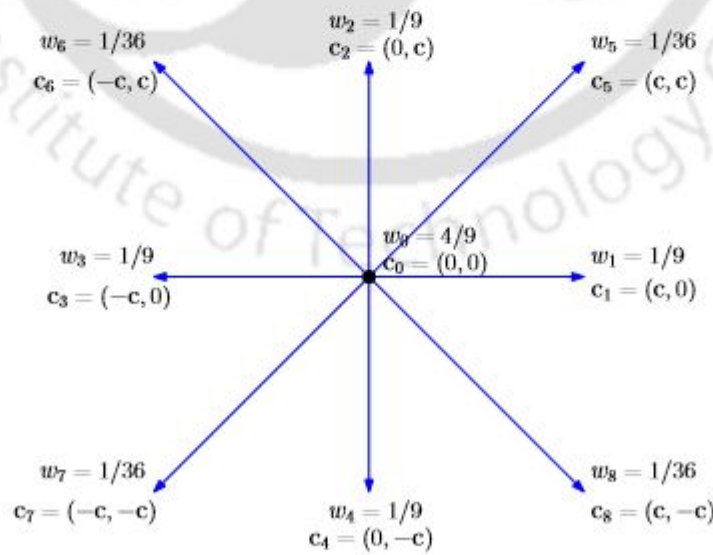


Figure 2.1: Schematic showing velocity directions ($\mathbf{c}_i$) and corresponding weights (w_i) for a D2Q9 lattice arrangement.

of state as shown in Eq. (2.6).

$$p = \rho_f c_s^2 \quad (2.6)$$

The hydrodynamic boundary conditions on plane surfaces at the LB level are realized through the non-equilibrium bounce-back method (popularly known as Zou/He) [11] in the present work.

2.1.1 Simplified Thermal Lattice Boltzmann Method

The thermal lattice-Boltzmann method (TLBM) for simulation of heat transfer processes can be broadly classified on the basis of the choice of distribution function as (1) the single population model (or multi-speed model), (2) the double population model, and (3) the hybrid model. Single population model [85] comprises only density distribution function with higher order velocity terms. The energy equation utilizes additional discrete velocities. The passive scalar model utilizes a separate distribution function to obtain the temperature field. It possesses higher numerical stability than the multi-speed model but lacks viscous dissipation and compression work terms. Similarly, in the double population model [22], an additional distribution function is considered for thermal LBE along with the density-distribution function to solve for momentum using isothermal LBE. The double population model also possesses advantages over the single population model in terms of numerical stability, narrow temperature range applications, and considering viscous dissipation and compression work. Simplified thermal LBE [23] is a case of a double population model corresponding to the energy equation without viscous heat dissipation term and compression work done by pressure. In the hybrid TLB model [63], the energy-forcing term is added to the simplified TLB equation by discretizing the macroscopic energy equation using the finite difference method, whereas the mass and momentum conservation are solved using the usual isothermal LB discretization.

The simplified thermal lattice-Boltzmann equation (STLBE) in a uniform lattice with single relaxation time BGK collision operator (Ψ_i^{BGK}) can be expressed as [23]

$$g_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - g_i(\mathbf{x}, t) = \Psi_i^{BGK} \quad (2.7)$$

$$\Psi_i^{BGK} = \frac{\Delta t}{\tau_{g,f}} [g_i^{eq}(\mathbf{x}, t) - g_i(\mathbf{x}, t)] \quad (2.8)$$

where g_i and g_i^{eq} is the energy distribution function and equilibrium energy distribution function along the particle velocity direction $\mathbf{c}_i$ for the temperature field ($T(\mathbf{x}, t)$) respectively. $\tau_{g,f}$ represents the dimensionless relaxation time for the STLBE. The

equilibrium energy distribution function in a D_2Q_9 lattice setup for incompressible thermal flows, can be determined as [22][23]

$$g_i^{eq} = \begin{cases} w_i \rho_0 T \left[-\frac{1}{2} \frac{(\mathbf{u} \cdot \mathbf{u})}{c_s^2} \right], & i = 0 \\ w_i \rho_0 T \left[\frac{3}{2} + \frac{1}{2} \frac{(\mathbf{c}_i \cdot \mathbf{u})}{c_s^2} + \frac{1}{2} \frac{(\mathbf{c}_i \cdot \mathbf{u})^2}{c_s^4} - \frac{1}{2} \frac{(\mathbf{u} \cdot \mathbf{u})}{c_s^2} \right], & i = 1, 2, 3, 4 \\ w_i \rho_0 T \left[3 + 2 \frac{(\mathbf{c}_i \cdot \mathbf{u})}{c_s^2} + \frac{1}{2} \frac{(\mathbf{c}_i \cdot \mathbf{u})^2}{c_s^4} - \frac{1}{2} \frac{(\mathbf{u} \cdot \mathbf{u})}{c_s^2} \right], & i = 5, 6, 7, 8 \end{cases} \quad (2.9)$$

The thermal diffusivity χ_f is related to the dimensionless relaxation time $\tau_{g,f}$ as,

$$\chi_f = 2(\tau_{g,f} - 0.5)c_s^2 \Delta t \quad (2.10)$$

The macroscopic temperature can be recovered by using

$$\rho_0 T = \sum_i g_i \quad (2.11)$$

In the present study, the coupling of energy and momentum equations is realized through the Boussinesq approximation of the body force term during natural and mixed convection problems. Boussinesq approximation assumes constant thermo-fluid properties (like density, viscosity, thermal diffusivity, etc.) except for the density involved in the body force term, which is again considered a linear function of temperature. Thus the buoyancy force term can be expressed as,

$$\mathbf{F}(\mathbf{x}, t) = \rho_0 \mathbf{g} \beta (T - T_0) \quad (2.12)$$

where $\mathbf{g}$ is the acceleration due to gravity, β is the coefficient of thermal expansion, and T_0 is the bulk fluid temperature. This body force density term can be incorporated in the SRT LBE using Guo's [72] discrete forcing term (F_i), and thus Eq. (2.1) is modified as

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = \frac{\Delta t}{\tau_f} [f_i^{eq}(\mathbf{x}, t) - f_i(\mathbf{x}, t)] + F_i \Delta t \quad (2.13)$$

$$F_i(\mathbf{x}, t) = \left(1 - \frac{1}{2\tau_f} \right) w_i \left[\frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^2} + \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^4} \right] \cdot \mathbf{F}(\mathbf{x}, t) \quad (2.14)$$

The fluid velocity used in Eq. (2.14) is constituted through a corrector step as

$$\rho_0 \mathbf{u}(\mathbf{x}, t) = \sum_i \mathbf{c}_i f_i + \frac{\Delta t}{2} \mathbf{F}(\mathbf{x}, t) \quad (2.15)$$

The temperature boundary conditions on the plane surfaces are applied using the methodology proposed by Liu et al. [86] in the present work.

2.2 Introduction to PSC

The fully explicit nature of the discretized LB equation, coupled with uniform grid, bestows an amiable numerical framework, conjoined with ease of parallelization, for problems involving complex boundaries. Conventional LB procedure, however, is applicable solely to the fluid domain, with bounce-back-like schemes being popularized for contriving the unknown distribution functions at the solid-fluid interfaces. While such an approach vouches for mass conservation and promises second-order accuracy, the quality of prediction of hydrodynamic forces at moving fluid-particle interfaces can be significantly degraded, often paired with spurious fluctuations of non-negligible amplitude. This necessitates the evolution of a generalized equation capable of uniformly delineating both fluid and solid behavior, with particular emphasis on precise emulation of the interfacial parameters for any intricate non-body-conforming grid scenario, while retaining the locality of the collision operator and linearity of the streaming exercise. This leads to the PSC approach, where the LB evolution equation [Eq. (2.1)] is augmented with an additional collision operator (Ω_i^B), facilitating the resultant governing equation to act as a weighted-average one pertaining to all components present within the purview of the domain, coupled with meticulous exertion of the boundary conditions. This newly-introduced solid collision operator treats each of the solid, fluid and interfacial cells distinctly based on the consequent magnitude of the solid volume fraction, and its evolution equation can be presented in accordance with Noble and Torczynski [45] as,

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \left[1 - \sum_S B(\Phi_B, \tau_f) \right] \Omega_i^{BGK} + \sum_S B(\Phi_B, \tau_f) \Omega_i^B + \left[1 - \sum_S B(\Phi_B, \tau_f) \right] F_i \Delta t \quad (2.16)$$

Here the solid volume fraction Φ_B local to a cell is computed as the cumulative contribution from each of the individual particles within the set S interacting at that specific node, while the local weight function $B(\Phi_B, \tau_f)$ is determined from Φ_B , as detailed later. The implementation of PSC approach, pioneered by Noble and Torczynski [45], is relatively straightforward for problems involving stationary interfaces requiring a one-time evaluation of Φ_B at every computational cells. For moving boundary situations, the solid fraction needs to be updated at every time instant, considering the particle kinetics and amended positioning. One of the most lucrative features of PSC over conventional LBM refers to this precise context, as it involves zero additional obligation to confront the continual birth and death of both fluid and solid nodes consequent to the particle motion. While contemplating the contributions from each of the

neighbors to a particular node during collision, all the adjoining cells will be suitably dealt with, thereby warranting mass and momentum conservation. The PSC approach eliminates the staircase nature of the bounce-back approach but does not exactly represent the solid boundary either, because only an averaged solid volume fraction is available. Nevertheless, this suffices to mitigate the momentum discontinuity at the interface for reasonable grid resolutions. The computation of the solid volume fraction and the solid collision operator specific to the present work and implementation of the PSC approach are detailed in the following subsections.

2.2.1 Computation of solid volume fraction

Appraisal of the solid volume fraction (Φ_B) is the central and most computation-intensive constituent of PSC, especially for moving-boundary problems, which compels re-assessment of Φ_B at every computational cell with each time advancement. The exact value of the volume fraction at the interface cells can be ascertained through simple geometric inferences, provided the particle assumes a uniform geometric silhouette. For configurations involving complex boundary or with deformable bodies, however, such approach can become circuitous, clamoring for a comprehensive and generalized solution. In the present study, the cell decomposition technique with the lattice nodes placed at the center of each computational cells throughout the domain is adopted. The volume fractions (Φ_B) for the interior solid cells (denoted by black color) and exterior fluid cells (denoted by white color) are initially demarcated as 1.0 and 0.0 respectively, as shown in Fig. 2.2. The computational cells accommodating the particle boundary are subsequently flagged as the interface cells (denoted by grey color), which are then subdivided into n_{sub}^2 equal-sized sub-squares. An inside-outside algorithm [87] is adopted to determine the number of sub-cells persisting interior to the particle boundary, thereby allowing the estimation of Φ_B as the ratio of the number of such interior sub-cells to the total number of sub-cells available in the concerned computational cell.

2.3 Partially Saturated Computational Cells Method for Momentum Equations

The evolution equation for momentum equations using PSC is expressed in Eq. (2.16). The weighting function $B(\Phi_B, \tau_f)$ can be modeled in two linear and non-linear versions viz., B1 and B2 as

$$\text{B1 :} \quad B(\Phi_B, \tau_f) = \Phi_B \quad (2.17a)$$

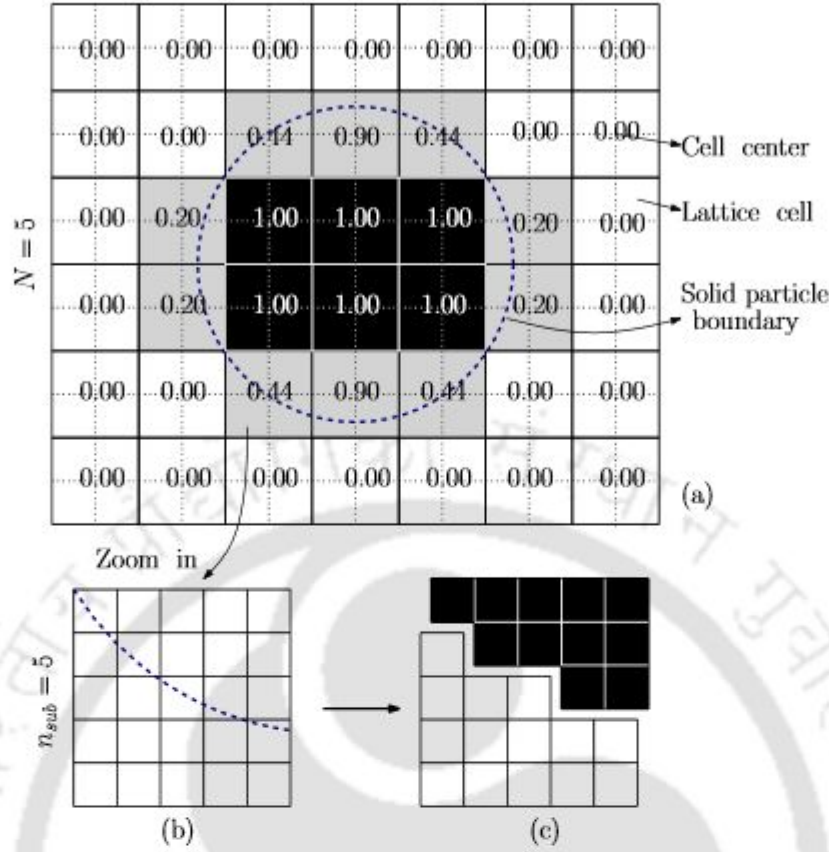


Figure 2.2: (a) PSC strategy of assigning Φ_B . Black, white and grey cells represent solid, fluid and interface cells respectively; (b) A partially saturated cell is zoomed in and decomposed into $n^2 = 25$ sub-cells; (c) Volume fraction of an interface cell (Φ_B) is the ratio of number of sub-cells covered by solid particle (represented by black color) to total number of sub-cells

$$\mathbf{B2}: \quad B(\Phi_B, \tau_f) = \frac{\Phi_B(\tau_f/\Delta t - 1/2)}{(1 - \Phi_B) + (\tau_f/\Delta t - 1/2)} \quad (2.17b)$$

It is evident that the weight function converges to zero and one for the respective limiting cases of pure fluid and pure solid cells, while maintaining a value within these two limits for the interface cells, as desired. With continuous rise in the relaxation time (τ_f), B approaches the solid volume fraction (Fig. 2.3). Such interface smoothing is imperative towards the success of the evolved LB algorithm, as it emulates the classical LB equations with standard BGK collision operator in the fluid domain and solid kinetic equation in the solid domain, and employs the weighted collision operator for the interface cells engaging the concerned solid volume fraction.

Two different forms for the solid collision operator (Ω_i^B) were proposed by Noble and Torczynski [45], as follows-

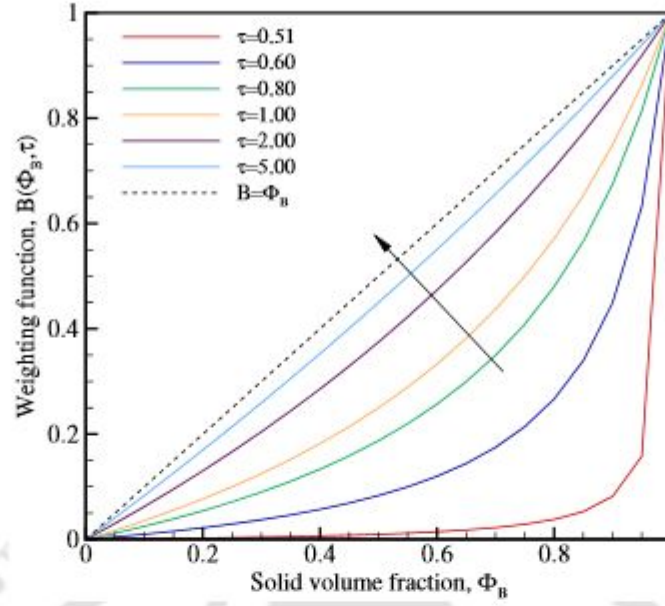


Figure 2.3: Variation of weighting function ($B(\Phi_B, \tau)$) as a function of solid volume fraction (Φ_B) for different values of τ .

Superposition model:

$$\Omega_i^B = f_i^{eq}(\rho_f, \mathbf{U}_p) - f_i(\mathbf{x}, t) + \left(1 - \frac{\Delta t}{\tau_f}\right) [f_i(\mathbf{x}, t) - f_i^{eq}(\rho_f, \mathbf{u})] \quad (2.18a)$$

Bounce back of non-equilibrium part/non-equilibrium reflection model:

$$\Omega_i^B = f_{-i}(\mathbf{x}, t) - f_i(\mathbf{x}, t) + f_i^{eq}(\rho_f, \mathbf{U}_p) - f_{-i}^{eq}(\rho_f, \mathbf{u}) \quad (2.18b)$$

While the former, utilizes the deviation of current distribution from its equilibrium, the latter accordant to its name, enforces the bounce-back of the non-equilibrium part of the distribution function at the limiting situation of pure solid. It also needs to be noted that the collision term tends to converge towards its equilibrium pattern with the time step equaling the relaxation time. Equation (2.18a) along with Eq. (2.17b) exhibits sublinear convergence with respect to grid resolution and lesser errors with increase in τ_f as compared to the latter variant of the collision operator [50] and therefore has been adopted for hydrodynamic simulations in the present study. In addition to it, the recovery of Navier-Stokes equations using the above-mentioned models through Chapman-Enskog analysis are elaborated in detail by Najuch and Sun [49]. Henceforth, the algorithm for the evaluation of momentum equations is referred to as the hydrodynamic-PSC method in this thesis.

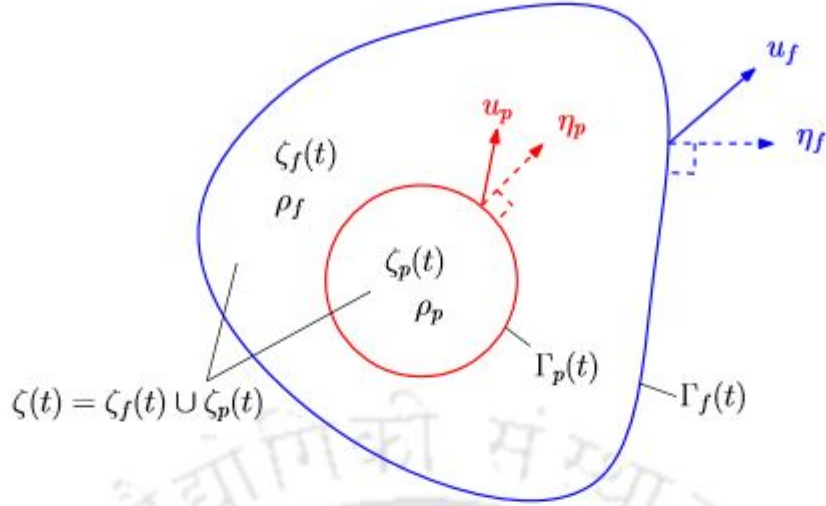


Figure 2.4: Time varying control surface ($\Gamma_p(t)$ and $\Gamma_f(t)$) and its corresponding control volumes ($\zeta_p(t)$ and $\zeta_f(t)$)

2.3.1 Incorporation of particle dynamics

Accurate evaluation of forces and moments on the solid (particle) due to the fluid is necessary in problems involving fluid-structure interaction. Traditional LB practices of apprising hydrodynamic forces like momentum exchange method [6, 88] and stress integration method [7] necessitates complicated and tedious interpolations of the particle distribution function to identify the magnitude at the interface. A moving boundary scenario instills further intricacy with the continuous fluid-to-solid and converse transformation of certain nodes, thereby requiring reconstruction of the distribution function, using methods like the refilling schemes [50], at every time-step. The PSC algorithm leads to substantial respite in this regard due to lesser number of interpolations and also leads to considerable smoothening in spurious fluctuations.

To understand the procedure of hydrodynamic force evaluation in the PSC approach, a solid particle of time-varying surface area $\Gamma_p(t)$ and volume $\zeta_p(t)$ is envisioned to be immersed into a time-dependent fluid control volume of surface area $\Gamma_f(t)$ and volume $\zeta_f(t)$, as detailed in Fig. 2.4. The arbitrary velocity directions and outward normal surface vectors for both the particle and control volume at any random instant are also shown there. Consequently, the net surface force exerted by the fluid over the particle ($f \rightarrow p$) can be estimated by integrating of the concerned forces over the complete surface of the particle as,

$$\mathbf{F}_{f \rightarrow p} = - \int_{\Gamma_p} [\rho \mathbf{u} (\mathbf{u} - \mathbf{u}_p) + \sigma] \cdot \boldsymbol{\eta}_p d\Gamma \quad (2.19)$$

with σ being the viscous stress tensor. The concerned fluid mass at this particular

instant can be considered to be constrained by the control surfaces Γ_p and Γ_f . Its conservation of linear momentum can, therefore, be presented following the Cauchy's stress principle as,

$$\frac{\partial}{\partial t} \int_{\zeta_f} \rho \mathbf{u} d\zeta = - \int_{\Gamma_f} [\rho \mathbf{u} (\mathbf{u} - \mathbf{u}_f) + \sigma] \cdot \boldsymbol{\eta}_f d\Gamma - \int_{\Gamma_p} [\rho \mathbf{u} (\mathbf{u} - \mathbf{u}_p) + \sigma] \cdot (-\boldsymbol{\eta}_p) d\Gamma \quad (2.20)$$

which can subsequently be combined with Eq. (2.19) to yield,

$$\frac{\partial}{\partial t} \int_{\zeta_f} \rho \mathbf{u} d\zeta = -\mathbf{F}_{f \rightarrow p} - \int_{\Gamma_f} [\rho \mathbf{u} (\mathbf{u} - \mathbf{u}_f) + \sigma] \cdot \boldsymbol{\eta}_f d\Gamma \quad (2.21)$$

The unified equation for the conservation of linear momentum for the complete domain encompassing both solid (ζ_p) and fluid volumes (ζ_f) can similarly be written as,

$$\frac{\partial}{\partial t} \int_{\zeta_f \cup \zeta_p} \rho \mathbf{u} d\zeta = - \int_{\Gamma_f} [\rho \mathbf{u} (\mathbf{u} - \mathbf{u}_f) + \sigma] \cdot \boldsymbol{\eta}_f d\Gamma + \int_{\zeta_f \cup \zeta_p} \mathbf{F} d\zeta \quad (2.22)$$

with $\mathbf{F}$ corresponding to the fluid-particle interaction force. Accordingly, an updated expression for the surface force acting on the particle owing to the momentum interaction with the fluid can be obtained by subtracting Eq. (2.21) from Eq. (2.22), as follows.

$$\mathbf{F}_{f \rightarrow p} = \underbrace{\frac{\partial}{\partial t} \int_{\zeta_p} \rho \mathbf{u} d\zeta}_{\text{added mass}} - \int_{\zeta_f \cup \zeta_p} \mathbf{F} d\zeta \quad (2.23)$$

A meticulous deliberation of the virtual mass (added mass) effect, appearing as the first term on the right-hand side of Eq. (2.23), is of acute importance in moving boundary problems. It corresponds to the augmentation in the inertia of the fluid neighboring to the body during its translocation, and hence relevant solely for accelerating particles and for fluid nodes in immediate proximity of the instantaneous interface. Incorporation of such ancillary acceleration is tricky as the general evolution equation is construed at all computational nodes, regardless of its topography relative to the interface. No-slip condition needs to be externally enforced at the surface, which emanates hypothetical fluid motion interior to the interface. The solid collision operator introduced in the evolution equation of PSC [Eq. (2.16)], however, can effortlessly distinguish fluid and solid nodes, consequently allowing evaluation of the interaction force at the interfacial nodes, and hence giving a better estimate of the virtual mass.

There are quite a few approaches available in the literature to emulate the fluid-particle interaction in immersed-boundary mode, such as Uhlmann's rigid body approximation [89], Feng's rigid body approximation [90] and Lagrangian points approx-

imation [91], to name a few. Despite being reasonably popular, Uhlmann's method has limited success for solid-to-fluid density ratio greater than 1.5, with the accuracy being reliant on problem configuration, mesh details and numerical scheme. The present work employs Feng's approach, which promises stable computation with no known restriction on density ratio. Accordingly, the added mass term of Eq. (2.23) is replaced by the acceleration experienced by a virtual fluid element having identical volume to the particle (ζ_p) and moving with its center-of-mass velocity ($\mathbf{u}_c$).

$$\mathbf{F}_{f \rightarrow p} = \rho \zeta_p \frac{\partial \mathbf{u}_c}{\partial t} - \int_{\zeta_f \cup \zeta_p} \mathbf{F} d\zeta \quad (2.24)$$

For a non-accelerating particle (stationary or moving with constant linear or rotational velocity), the first term on the right-hand side of the above equation vanishes, reducing the force evaluation procedure to a simple numerical integration of boundary forces, regardless of the position of the particle.

$$\int_{\zeta_f \cup \zeta_p} \mathbf{F} d\zeta \approx \sum \mathbf{F} \Delta x^D \quad (2.25)$$

where D stands for the dimension of the problem. The motion of the particle needs to be tracked in the PSC framework for the appraisal of the virtual mass formulation, which can be realized by solving the Newton's linear and angular momentum conservation equations for the particle itself. Accordingly, the translational velocity can be traced as,

$$\rho_p \zeta_p \frac{d\mathbf{u}_c}{dt} = -\mathbf{F}_{f \rightarrow p} + (\rho_p - \rho_f) \zeta_p \mathbf{g} + \mathbf{F}^c \quad (2.26)$$

where $\mathbf{F}^c$ corresponds to the particle-particle and particle-wall collision, which is conceived following Feng et al. [40]. Conservation of angular momentum can be achieved by taking a moment over Eq. (2.26), while neglecting $\mathbf{F}^c$ in the present study, as

$$I_p \frac{d\Omega_p}{dt} = \frac{\partial}{\partial t} \int_{\zeta} (\mathbf{x}_p - \mathbf{x}_c) \times \rho_f \mathbf{u}_c d\zeta - \int_{\zeta} (\mathbf{x}_p - \mathbf{x}_c) \times \mathbf{F} d\zeta \quad (2.27)$$

where I_p , Ω_p , $\mathbf{x}_p$ and $\mathbf{x}_c$ are mass moment of inertia, angular velocity, position vectors of the interfacial point and the reference point respectively. Also note that the first term on the right-hand side is the manifestation of the added mass effect of a rigid body having non-uniform angular velocity. Once the particle motion is completely described, its position and surface velocity can regularly be updated as,

$$\frac{d\mathbf{X}_c}{dt} = \mathbf{u}_c \quad (2.28a)$$

$$\mathbf{u}_p(\mathbf{X}_p) = \mathbf{u}_c + \Omega_p \times (\mathbf{X}_p - \mathbf{X}_c) \quad (2.28b)$$

The first-order Euler explicit method is utilized for numerically evaluating the temporal derivatives of Eqns. (2.26), (2.27) and (2.28a), while the new interfacial force and torque are resolved considering momentum transfer involving each of the solid nodes as [46],

$$\mathbf{F} = \frac{\Delta x^D}{\Delta t} \sum_{\forall \Phi_B > 0.0} B \sum_k \Omega_k^B c_k \quad (2.29a)$$

$$\mathbf{T} = \frac{\Delta x^D}{\Delta t} \sum_{\forall \Phi_B > 0.0} (\mathbf{X}_p - \mathbf{X}_c) \times B \sum_k \Omega_k^B c_k \quad (2.29b)$$

with k being the lattice velocity directions. The complete numerical procedure of the PSC algorithm which has been implemented in the indigenous in-house solver is summarized in Algorithm 1.

Algorithm 1: Computational steps for partially saturated computational cell (PSC)-based lattice Boltzmann method

```

Grid generation;
Initialization;
for each time step  $t$  do
    Obtain solid volume fraction  $\Phi_B$  and weighting function  $B$  values at each cell;
    Apply PSC governing equations via collision and streaming steps along with the evaluation of solid collision operator for each cell [Eq. (2.18b) or Eq. (2.18a)];
    Apply boundary condition at domain boundaries;
    Evaluate macroscopic variables using Eqns. (2.4a) and (2.4b);
    Obtain total force [Eq. (2.29a)] and torque [Eq. (2.29b)] on the particle;
    Calculate translational [Eq. (2.26)] and angular velocities of the particle [Eq. (2.27)];
    Update particle location  $\mathbf{X}_c$  using Eq. (2.28a);
    Obtain desired particle velocity  $\mathbf{U}_p$  on the surface of the particle using Eq. (2.28b);
end

```

2.4 Partially Saturated Computational Cells Method for Energy Equations

PSC methodology for heat transfer problems [80], likewise the hydrodynamic-PSC, also offers a unified evolution equation for solid and fluid media present in a computational domain. The augmentation of an additional solid collision operator (Ψ_i^B) to STLBE [Eq. (2.7)], along with a volume of solid (Φ_B) based weighting function [$B_t(\Phi_B, \tau_{g,f})$] provides accurate implementation of Dirichlet type temperature boundary conditions

over the immersed surface. The evolution equation of the method, hereafter referred to as thermal-PSC, is represented as,

$$g_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - g_i(\mathbf{x}, t) = \left[1 - \sum_S B_t(\Phi_B, \tau_{g,f}) \right] \Psi_i^{BGK} + \sum_S B_t(\Phi_B, \tau_{g,f}) \Psi_i^B \quad (2.30)$$

In addition to smooth diffusion of the boundary conditions at the solid-fluid interface, thermal-PSC retains the locality of collision operations and the linearity of streaming inherent to LB philosophy. Moreover, the method offers several advantages over the conventional STLBE methodology like the elimination of staircase-like representation of solid-fluid interface, no ancillary treatment for continuous birth and death of solid and fluid cells during particle motion, and smoother representation of force and temperature signals. In the present work, the additional collision operator introduced by Chen and Müller [80] is inducted in Eq. (2.30).

$$\Psi_i^B = -g_{-i}(\mathbf{x}, t) - g_i(\mathbf{x}, t) + g_i^{eq}(\rho_f, \mathbf{U}_p, T_p) + g_{-i}^{eq}(\rho_f, \mathbf{u}, T) \quad (2.31)$$

The mathematical formulation of weighting function $[B_t(\Phi_B, \tau_{g,f})]$ utilized in Eq. (2.30) is analogous to that expressed in Eqns. (2.17), and can be written as,

$$\mathbf{B1} : \quad B_t(\Phi_B, \tau_{g,f}) = \Phi_B \quad (2.32a)$$

$$\mathbf{B2} : \quad B_t(\Phi_B, \tau_{g,f}) = \frac{\Phi_B(\tau_{g,f}/\Delta t - 1/2)}{(1 - \Phi_B) + (\tau_{g,f}/\Delta t - 1/2)} \quad (2.32b)$$

Rettinger and Rude [50] reported that the combination of Eq. (2.18b) and B1 [Eq. (2.17a)] lacks in terms of accuracy whereas the combination of Eq. (2.18a) and B2 [Eq. (2.17b)] is recommended to obtain reasonably accurate results in hydrodynamic problems. Present simulations also reveal that the combination of Eqns. (2.18b), (2.31) and B2 [Eqns. (2.17b) and (2.32b)] outperforms the accuracy of results that utilize the B1 model. Nevertheless, the results comprising B1 combinations are not included to maintain the brevity of the thesis. Henceforth, the present work utilizes Eqns. (2.17b), (2.18b), (2.31) and (2.32b) for all the thermal simulations presented in chapter 4. Additionally, the fluid properties like density and viscosity are assumed to be constant, uniform, and independent of temperature in the present simulations. The viscous dissipation due to heat is also considered to be negligibly small. Such assumptions are adopted in many studies [61, 63, 73], pertaining to thermal immersed boundary methods, and can be regarded as valid for problems investigated in the present work. The recovery of the macroscopic energy equation from the thermal-PSC

governing Eq. (2.30) is elucidated in the Appendix A.

2.4.1 Procedure for calculation of local Nusselt number

Spurious force oscillations are inevitable during any particle motion in a flow field, and its investigation is an important aspect of immersed boundary methods. The present thesis quantifies the dependence of such oscillations as a function of grid resolution using hydrodynamic-PSC in Section 3.3. Likewise, the determination of temperature gradient on any complex arbitrary surface of an immersed body is an effortful task. Since the surface of immersed bodies is not aligned with the underlying regular Cartesian lattice mesh, and in particular, there is no sharp representation of the surface, obtaining a normal gradient of temperature on this surface becomes arduous. In the present work a mechanism to obtain local temperature gradient on any arbitrary shape is devised, which is inspired by the Eulerian-Lagrangian computational framework. The appraisal of local Nusselt number (Nu) using this mechanism for the thermal-PSC algorithm is a novel aspect of the present study which was not forthcoming in the available literature. Let us consider an arbitrary surface immersed into an Eulerian flow field as shown in Fig. 2.5. The immersed surface is divided into a finite number of Lagrangian nodes. Here, $\mathbf{X}_b$ and $\mathbf{x}$ represent position vectors of Lagrangian and Eulerian nodes, respectively. Let, $\mathbf{h}(\mathbf{X}_b, t)$ be heat flux vector such that $\mathbf{h} = \hat{i}\mathbf{h}_x + \hat{j}\mathbf{h}_y$ and $\mathbf{X}_b = \hat{i}\mathbf{x}_b + \hat{j}\mathbf{y}_b$. Supposing that, $g_i(\mathbf{x}, t)$ and $T(\mathbf{x}, t)$ are known,

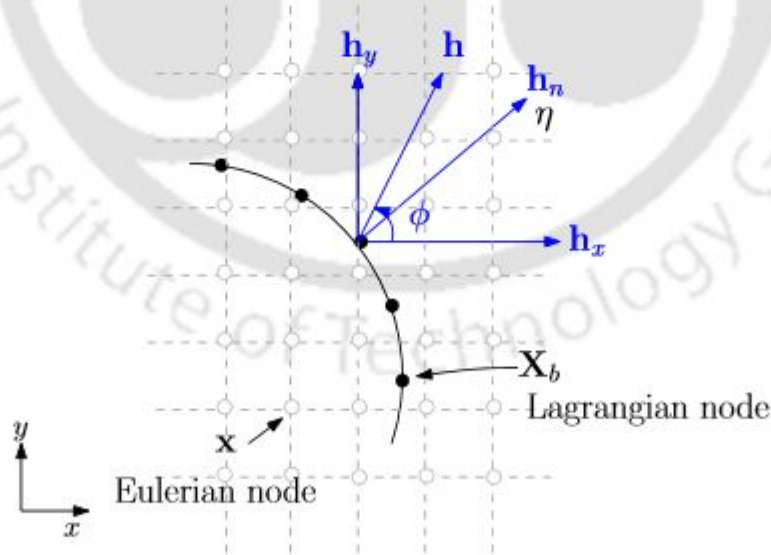


Figure 2.5: Schematic showing an arbitrary surface having Lagrangian nodes immersed into a flow field having Eulerian points.

heat flux vector at Eulerian nodes can be evaluated as,

$$\mathbf{h}(\mathbf{x}, t) = -k_f \nabla T \quad (2.33)$$

The temperature gradient in Eq. (2.33) is obtained using a second-order accurate finite difference scheme, and the thermal conductivity of fluid at the LB level is given as [73]

$$k_f = \frac{1}{3} \tau_{g,f} \Delta x \quad (2.34)$$

The heat flux vector at the Lagrangian nodes can now be obtained by interpolating heat flux from Eulerian nodes using the Dirac-delta function.

$$\mathbf{h}(\mathbf{X}_b, t + \Delta t) = \sum \mathbf{h}(\mathbf{x}, t + \Delta t) D(\mathbf{x} - \mathbf{X}_b) h^2 \quad (2.35)$$

where, h represents mesh spacing and $D(\mathbf{r})$ is a continuous kernel distribution which approximates Dirac-delta function $\delta(\mathbf{r})$ as,

$$D(\mathbf{x} - \mathbf{X}_b) = \frac{1}{h^2} \delta\left(\frac{x - X_b}{h}\right) \delta\left(\frac{y - Y_b}{h}\right) \quad (2.36)$$

For a two-dimensional coordinate system, $\delta(\mathbf{r})$ can be formulated as,

$$\delta(r) = \begin{cases} \frac{1}{4} \left[1 + \cos\left(\frac{\pi r}{2}\right) \right] & |r| \leq 2 \\ 0 & |r| > 2 \end{cases} \quad (2.37)$$

Thus, the normal heat flux vector along the unit normal to the surface (η) is evaluated as

$$\mathbf{h}_n(\mathbf{X}_b, t + \Delta t) = \eta \cdot \mathbf{h}(\mathbf{X}_b, t + \Delta t) \quad (2.38)$$

The local and averaged Nusselt number over the surface of a circular cylinder having diameter d , is determined as

$$Nu(\theta) = \frac{h_n(\theta)}{k_f (\Delta T/d)} \quad (2.39)$$

$$\overline{Nu} = \frac{1}{\pi d} \int_0^{2\pi} Nu(\theta) \frac{d}{2} d\theta \quad (2.40)$$

Here, ΔT represents characteristic temperature difference. The magnitude of temperature in the present work is non-dimensionalized across all the test cases. Previously, inverse distance weighting and staircase approximation of the immersed surface have been used by De [83] and Kumar and Natarajan [87] respectively, during the evaluation of the local Nusselt number in the finite-volume counterpart of the diffuse interface-

immersed boundary method. Suzuki et al. [73] proposed a correction-based heat-flux calculation technique comprising energy distribution function. The preliminary results reveal that the present methodology yields a comparable variation of the local Nusselt number as compared to the aforementioned techniques in the thermal-PSC method. Highly spurious signals of temperature gradients are inevitable pertaining to the diffuse-interface IB methods. Thus, a smoother distribution of these gradients are presented by passing them through a low-pass filter. It must be mentioned here that Ren et al. [92] utilized the temperature gradient on Lagrangian nodes akin to the present methodology in a velocity and heat correction based finite difference-immersed boundary method as a part of its solution procedure. However, in the present work, the heat flux vector at Lagrangian nodes is solely used in post-processing, and they are never a part of the solution process of the thermal-PSC algorithm. The computational

Algorithm 2: Computational steps for hydrodynamic and thermal-PSC method

```

Grid generation;
Initialization;
for each time step  $t$  do
    Reconstruct the immersed body and evaluate volume fraction ( $\Phi_B$ ) and
    weighting functions ( $B$  and  $B_t$ ) using Eqns. (2.17) and (2.32);
    Obtain discrete forcing term using Eq. (2.14);
    Apply hydrodynamic-PSC governing Eq. (2.16), via collision and
    streaming operations;
    Apply hydrodynamic boundary conditions at domain boundaries following
    Zou and He [11];
    Evaluate macroscopic density and velocity using Eqns. (2.4a) and (2.4b)
    respectively ;
    Apply thermal-PSC governing Eqns. (2.30), via collision and streaming
    operations;
    Apply thermal boundary conditions at domain boundaries following Liu et
    al. [86];
    Evaluate macroscopic temperature ( $T$ ) using Eq. (2.11) ;
    Obtain total hydrodynamic forces and torque on the particle following
    Eqns. (2.29a) and (2.29b) respectively;
    Evaluate body force density using 2.12 (applicable for natural and mixed
    convection problems);
    Calculate translational [Eq. (2.26)] and angular velocities of the particle
    [Eq. (2.27)];
    Update particle location  $\mathbf{X}_c$  using Eq. (2.28a);
    Obtain desired particle velocity  $\mathbf{U}_p$  on the surface of the particle using Eq.
    (2.28b);
    Modify fluid velocity using a corrector step as 2.15.
end

```

steps of the present thermal-PSC methodology are outlined in the Algorithm 2.

In the subsequent chapters of the thesis, the aforementioned evolution equations and the post processing techniques will be utilized to investigate various numerical aspects and validate the in-house solver for a wide spectrum of fluid-particle interaction problems.



CHAPTER 3

REVISITING THE PSC METHOD FOR HYDRODYNAMIC STUDIES

“To really learn CFD, you must get your hands dirty; i.e; you must wade into the calculations and do them yourself”

- John D. Anderson, Jr., 1995

The present chapter revisits the hydrodynamic-PSC method in the context of incompressible single-phase flows past stationary and moving bodies. The focus of the chapter targets four facets - numerical accuracy, discrete conservation, spurious force oscillations, and benchmarking the methodology for a wide range of stationary and moving boundary problems. The study proves that the PSC approach exhibits nominal second-order accuracy in presence of straight and curved boundaries for pressure, although spatial order of accuracy in velocity degrades to first-order. The analysis also reveals that PSC is approximately discretely conservative in the incompressible limit with the mass conservation errors being dependent on the lattice size and relaxation time. For simulations involving moving body problems, the method is found to introduce acceptable level of spurious force oscillations, which rapidly decrease with increasing grid resolution. Extensive numerical experiments are performed involving both stationary and moving bodies, with imposed and induced motion, to assess the applicability of the PSC approach. The findings of the study illustrate that the inclusion of added mass effects are important for accurate force and torque computations

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in case of accelerating solids. Numerical investigations, that include unsteady flows featuring three degrees-of-freedom fluid-particle interactions clearly highlight the ability of the PSC approach in resolving complex hydrodynamical phenomena. This in-depth evaluation of the PSC approach conclusively demonstrates its efficacy as a promising computational framework for efficient and robust computations of incompressible fluid flows over a range of flow scenarios.

The PSC approach combines the simplicity of the underlying LB algorithm with a unified evolution equation [Eq. (2.16)] based on the solid volume fraction and an associated solid collision operator, thereby acting like an LB analogue of the volume-of-solid immersed boundary method in the finite volume framework [81, 82], to devise a robust and accurate methodology for fluid-structure interactions. The comprehensive survey of PSC literature in Chapter 1 reveals some studies associated with the accuracy [46, 47]. However, no known studies can be found that discuss the ability of the PSC approach to conserve mass and momentum at the discrete level and the performance of this technique for computing temporal histories of force coefficients when moving geometries are encountered. Hence the present chapter investigates these facets of the algorithm to establish its proficiency for simulation of incompressible hydrodynamic flows. The remainder of the chapter is organized as follows. Section 3.1 presents the accuracy of the hydrodynamic-PSC algorithm subjected to stationary and moving curved boundary problems. The discrete conservation and spurious force oscillations (SFO) of PSC are dealt in detail in Sections 3.2 and 3.3, respectively. Finally, the Section 3.4 demonstrates the efficacy of the PSC algorithm by validating the solver for a wide range of non-trivial benchmark curved boundary problems involving stationary and moving boundary scenarios. While the PSC is a simple-to-implement and promising approach in principle, the studies presented in this chapter shed light on aspects of the methodology that have hitherto not been explored in literature but are important for the practical viability of the approach.

3.1 Accuracy study

3.1.1 Taylor-Green decaying vortex

The well-known unsteady flow configuration of Taylor-Green decaying vortex in a square domain is contemplated as the first test case, where the following analytical velocity and pressure solutions are available in space and time, thereby providing a

direct option of assessing the numerical accuracy of the proposed solver.

$$u(x, y, t) = -U \cos(kx) \sin(ky) e^{-2\nu k^2 t} \quad (3.1a)$$

$$v(x, y, t) = U \sin(kx) \cos(ky) e^{-2\nu k^2 t} \quad (3.1b)$$

$$p(x, y, t) = -\frac{U^2}{4} [\cos(2kx) + \cos(2ky)] e^{-4k^2 \nu t} \quad (3.1c)$$

where $k = \pi/d$, d being the associated length-scale. A concentric circle of diameter d is artificially embedded into the computational domain of size $[2d \times 2d]$, for the purpose of investigating the order of accuracy, and it must be remarked that this configuration does not alter the flow. The Reynolds number ($Re = Ud/\nu_f$) and lattice-level relaxation time (τ_f) are fixed as 10 and 0.65 respectively. Time-dependent analytical solutions and periodic boundary conditions are adopted at immersed and domain boundaries respectively, whereas the domain is initialized with the analytical solutions at $t = 0$. The spatial accuracy is envisaged by considering four different numbers of grids across the diameter, *viz.*, 10, 20, 40 and 80 at a fixed $\tau_f = 0.65$.

The effect of grid resolution on the pressure and velocity error norms are illustrated in Fig. 3.1a, as the L_∞ norm for both are clearly second-order-accurate, demonstrated further by observing the slope of the concerned dashed line. Selection of relaxation time τ_f is also a key parameter in ensuring numerical accuracy, the effect of which can be analyzed from Fig. 3.1b. The numerical test is carried out by fixing the number of grids along the diameter equal to 20. The pressure and velocity

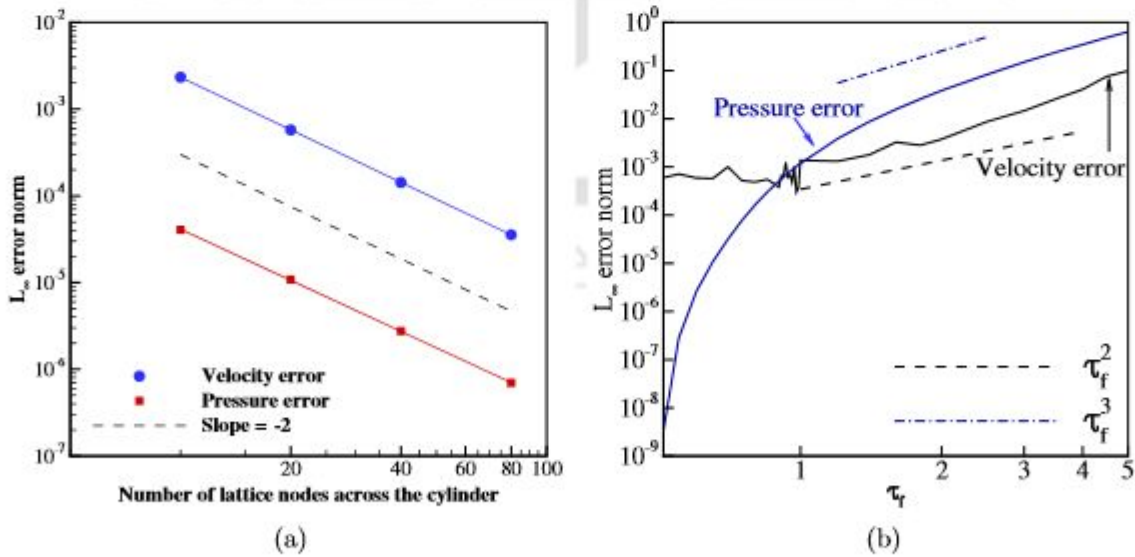


Figure 3.1: Variation of L_∞ errors with respect to (a) number of grids across the cylinder and (b) relaxation time (τ_f).

errors quantified by the L_∞ -norms decrease with τ_f adhering roughly to second- and third-order decay, and drops below the tolerable limit of 10^{-3} for $\tau_f < 1$.

3.1.2 Taylor-Couette problem

The flow solver is now tested with the Taylor-Couette flow where, unlike the previous subsection, an analytical solution is not imposed over the domain. Two concentric cylinders of radii $R_1 = 0.2L$ and $R_2 = 0.4L$ are embedded into a computational domain of size $L \times L$, as shown in Fig.3.2. The inner cylinder is rotating with a constant angular velocity $\Omega_P = U/R_1$, while the outer cylinder remains stationary. No-slip and impermeable wall boundary conditions are imposed over the shaded solid zones, restricting the flow within the annulus. Corresponding steady-state analytical solutions are of the following form.

$$u(x, y) = -\frac{\Omega_P R_1^2}{R_2^2 - R_1^2} \left(\frac{R_2^2}{r^2} - 1 \right) y \quad (3.2a)$$

$$v(x, y) = -\frac{\Omega_P R_1^2}{R_2^2 - R_1^2} \left(\frac{R_2^2}{r^2} - 1 \right) x \quad (3.2b)$$

$$p(x, y) = \left[\frac{\Omega_P R_1^2}{(R_2^2 - R_1^2)} \right]^2 \left\{ \frac{r^2}{2} - \frac{R_2^4}{2r^2} - R_2^2 \log(r^2) \right\} \quad (3.2c)$$

$$T = -4\pi\rho\nu_f \left[\frac{\Omega_P R_1^2 R_2^2}{R_2^2 - R_1^2} \right] \quad (3.2d)$$

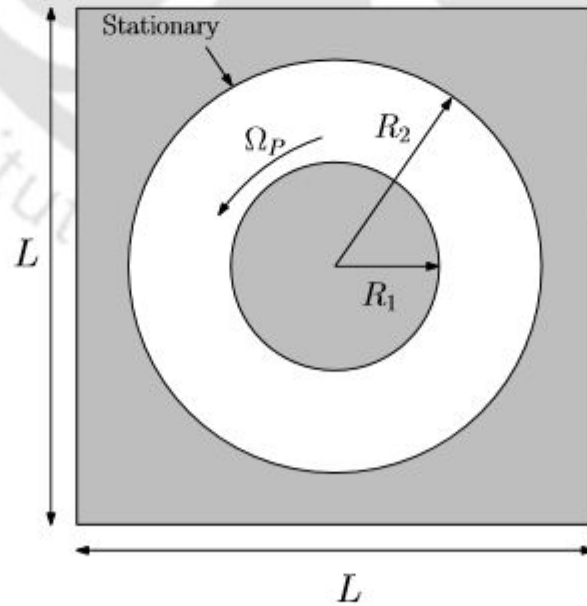


Figure 3.2: Computational domain for Taylor-Couette problem.

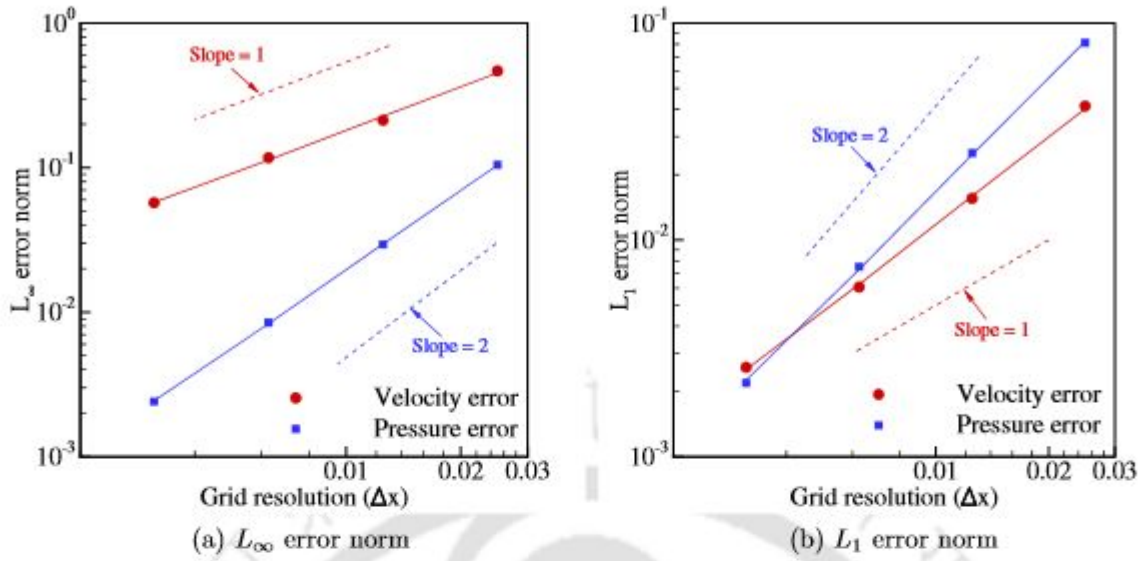


Figure 3.3: Spatial accuracy test of Taylor-Couette problem: (a) L_∞ and (b) L_1 error norms for velocities and pressure

where $r = \sqrt{x^2 + y^2}$ is the position vector and T represents the driving torque associated with the rotary motion.

To analyze the spatial accuracy in present problem, four different grid resolutions are considered, namely, $\Delta x = L/40, L/80, L/160, L/320$, while maintaining identical $Re = U(2R_1)/\nu_f = 50$, $\tau_f = 0.6$ and convergence criterion of 10^{-10} . Variation in corresponding error norms with grid spacing is summarized in Fig. 3.3. Both L_1 and L_∞ norms exhibit monotonic convergence with first-order accuracy (approximate slope of about 1.34 and 0.99 respectively), with the former being about one order smaller than the latter. A similar first order decline in velocity error was also reported by Owen *et al.* [48]. It is interesting to note here the degradation in the accuracy of velocity prediction from second-order in the previous case, where the imposition of exact boundary conditions inside the solid is possible, to first-order in the present moving-boundary problem. The pressure error, however, continues to have a second-order decline, with an approximate slope of 1.8 in this case. Excellent degree of conformity is also obtained in the velocity profiles with the exact solution (Fig. 3.4) which substantiates the capability of the PSC approach in dealing with moving and non-grid-conforming boundary. A further evidence of the competence of the approach can be found in the quantitative comparison of the simulated value of torque with its exact magnitude, as presented in Table 3.1. The reduction in relative torque error with grid refinement, which is also nearly first order, clearly highlights that the approach is also able to compute integrated hydrodynamic quantities accurately.

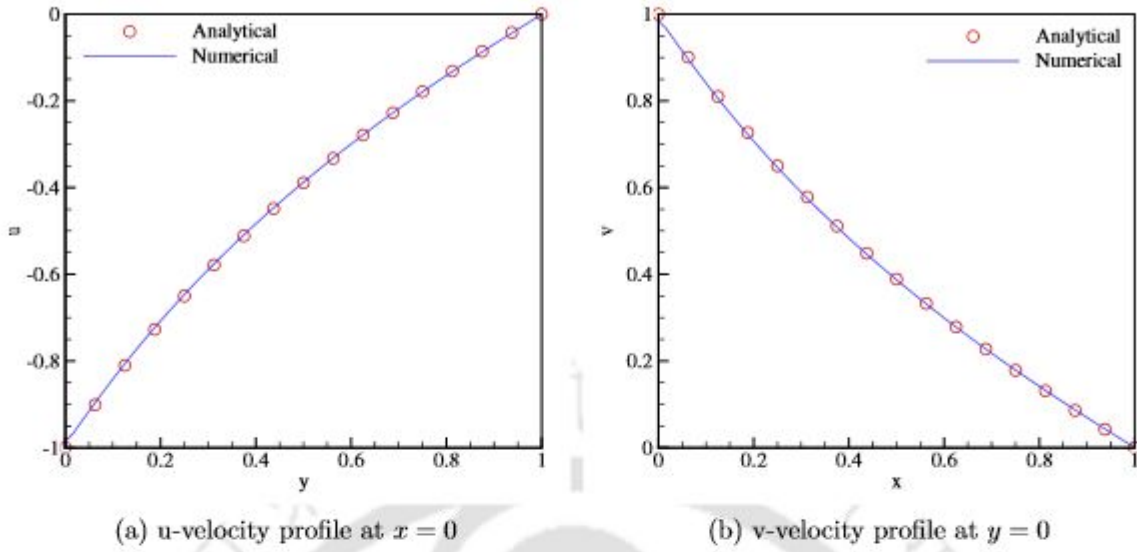


Figure 3.4: Comparison of numerical and analytical solutions of velocity profiles: (a) u-velocity profile at $x = 0$ and (b) v-velocity profile at $y = 0$

Table 3.1: Relative % error of the torque with respect to analytical solution ($T^{\text{analytical}} = -0.4654$) for different grid resolutions.

Δx	$T^{\text{numerical}}$	Relative % error
$1/40$	-0.4380	5.905
$1/80$	-0.4511	3.072
$1/160$	-0.4583	1.540
$1/320$	-0.4621	0.703

3.2 Discrete conservation study

The apprehension over the lack of mass conservation [93] is among the long-standing concerns with conventional LBM and it is therefore logical to explore the conservation properties of the PSC framework which is atleast first-order accurate. A solid computational domain of size $L \times L$ is considered, with one-fourth of an annular flow passage, having inner and outer radii of $0.7L$ and $0.9L$ respectively, immersed into it (Fig. 3.5a). This curved flow domain is subjected to a uniform velocity inlet (with $Re = 10$, defined based on annular gap), and constant pressure and zero normal velocity gradient at the exit. Figure 3.5b reveals that the local maximum divergence over the entire computational domain is confined to the order of 10^{-4} , which is an acceptable mass conservation error in most numerical setups. It is pertinent to mention here that the LBE algorithm (and hence PSC) is inherently susceptible to density fluctuations

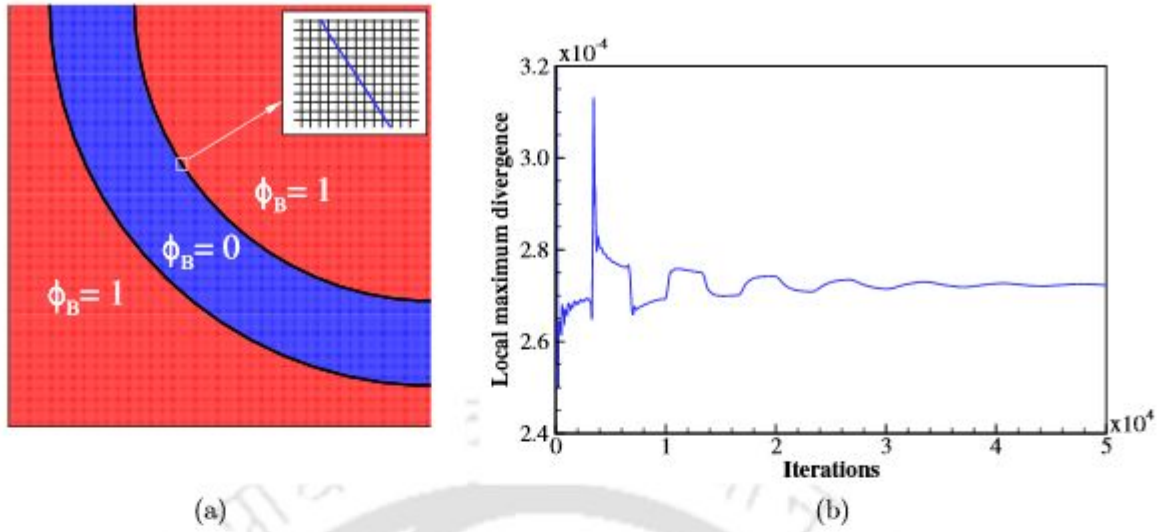


Figure 3.5: (a) Schematic representation of the computational domain with a flow through curved channel and its corresponding volume fraction (Φ_B) and (b) time evolution of local maximum divergence in the entire computational domain

emerging from the compressibility effect, which is the manifestation of density variation and velocity divergence source term present in the recovered Navier-Stokes' equation from the LBE while adopting the *pseudo-equation of state* $p = \rho c_s^2$, thereby deviating from true incompressible nature in classical mechanics sense [94]. These effects are negligible if density variations are small and thermodynamic considerations are not significant. The mass defect for the present problem and maximum density fluctuation over the entire domain encountered for multiple combinations of grid spacing and relaxation time are listed in Table 3.2. It is fairly evident that with the increasingly finer grid structure, both these quantities decrease considerably. The magnitude of $\Delta\rho_{max}$ also assures about inconsequential compressibility effect during simulations. With increase in relaxation time, however, the mass defect initially reduces and then rises to a significantly higher level, while the density fluctuations are continually amplified, thereby necessitating a careful and optimized selection of τ_f . Such a trend can be attributed to the strong dependence of the solid collision operator on the relaxation time and can possibly be highlighted as one of the limitations of the PSC methodology. Similar viscosity-dependent nature of the relative errors in force estimation and perturbed convergence behavior using PSC were also reported by Rettinger and R  de [50]. Another important point to be noted is the negligible velocity magnitude outside the flow domain, affirming adherence to the no-slip boundary condition within the solid and absence of any hypothetical flow initiation despite the channel boundaries being non-aligned to the underlying Cartesian mesh structure. This study affirms that the PSC approach guarantees approximate discrete mass conservation and is arguably

the first known demonstration of this fact.

Table 3.2: Mass flux defect and maximum density fluctuation for varying grid and τ_f

	Mass flux defect $ \dot{m}_{in} - \dot{m}_{out} $	Maximum density fluctuation $(\Delta\rho)_{max}$
Variable grid resolution ($L \times L$) for $\tau_f = 0.6$		
250×250	1.75×10^{-3}	1.98×10^{-3}
500×500	1.34×10^{-3}	7.75×10^{-4}
750×750	1.00×10^{-3}	4.68×10^{-4}
Variable relaxation time (τ_f) for grid resolution of 250×250		
0.60	1.75×10^{-3}	1.98×10^{-3}
0.70	5.57×10^{-4}	7.15×10^{-3}
0.80	5.86×10^{-3}	1.58×10^{-2}
0.90	1.97×10^{-2}	2.73×10^{-2}

3.3 Spurious force oscillations study

Another facet of paramount importance in simulation of moving-boundary problems is the encroachment of spurious oscillations during interfacial force estimation. It, though, has hardly received any attention under the purview of IB-LB approaches in general and possibly none with the PSC approach. In order to substantiate the efficacy of the PSC algorithm for moving body problems and fluid-structure interaction in particular, it is an absolute must to elucidate its performance in this particular front. To facilitate the study, an oscillatory motion of a circular cylinder within an initially quiescent domain of size $4d \times 4d$ is considered. The cylinder of diameter d is forced to oscillate in the x -direction about the domain center and its motion is described as,

$$X_c(t) = X_{c0} + A[1 - \cos(2\pi ft)] \quad , \quad u_c(t) = U_0 \sin(2\pi ft) \quad (3.3)$$

where, X_{c0} , A , f and U_0 are initial position of the cylinder, amplitude and frequency of oscillation and maximum cylinder velocity respectively. $A = 0.05d$, and corresponding Reynolds number ($Re = U_0 d / \nu_f$) and Strouhal number ($St = f d / U_0$) are set as 31 and 3.2 respectively following Seo and Mittal [95]. Neumann boundary condition with zero velocity gradient is realized at each of the domain boundaries adopting the non-equilibrium bounce-back (NEBB) approach[11]. For a quantitative assessment of the spurious force oscillations, it is necessary to first understand the numerical procedure towards interfacial force estimation. Referring to Fig. 3.6, F_x and F_y represent the x - and y -components of the resultant force, conventionally identified as drag and lift,

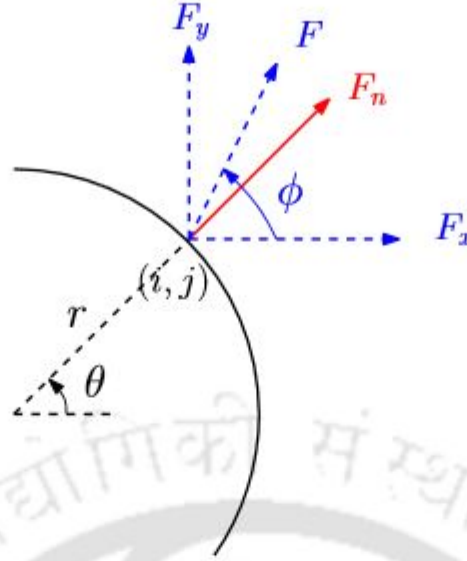


Figure 3.6: Schematic showing pressure force calculation.

while the net force $\mathbf{F} = \sqrt{F_x^2 + F_y^2}$ makes an angle ϕ with the horizontal and can be quantified using Eq. (2.29a). Both the components of $\mathbf{F}$ can separately be appraised using the vector descriptions of all c_k s involved in D_2Q_9 lattice configuration (Fig. 2.1). The pressure force at that particular (x, y) interfacial location can subsequently be evaluated by realizing the outward normal component of this resultant as,

$$F_{n(i,j)} = F_{i,j} \sin(\pi/2 - \phi + \theta) \quad (3.4)$$

with $\theta = \tan^{-1}(y/x)$. Net aerodynamic forces and concerned coefficients can accordingly be achieved as,

$$F_x = \sum_{\forall \Phi_{B,i,j} > 0.0} F_{x(i,j)}, \quad F_y = \sum_{\forall \Phi_{B,i,j} > 0.0} F_{y(i,j)}, \quad F_n = \sum_{\forall \Phi_{B,i,j} > 0.0} F_{n(i,j)} \quad (3.5a)$$

$$C_d = \frac{F_x}{0.5\rho u^2 d}, \quad C_l = \frac{F_y}{0.5\rho u^2 d}, \quad C_{PD} = \frac{F_n}{0.5\rho d^3 f^2} \quad (3.5b)$$

It must be remarked that a different non-dimensionalization for C_{PD} is employed as compared to C_d but that does not alter the conclusions arrived herein. Following the approach of Seo and Mittal [95], spurious fluctuations are comparatively more significant in pressure transients than the viscous forces and may be quantified using the 2δ -discontinuity in the temporal history of the pressure drag coefficient as,

$$C_{PD}^{2\delta} = |C_{PD}^{m+1} - 2C_{PD}^m + C_{PD}^{m-1}| \quad (3.6)$$

with n being time-step index.

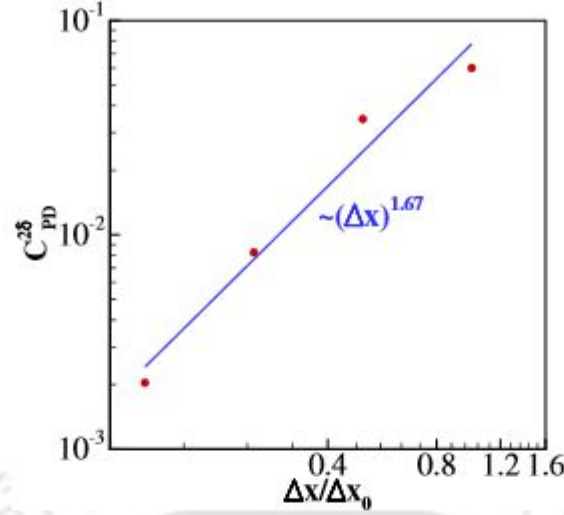


Figure 3.7: Variation of $C_{PD}^{2\delta}$ discontinuity with respect to the grid resolution.

Simulations are performed on a sequence of progressively refined grids following the sequence of $\Delta x/d = 1/16, 1/32, 1/64$, and $1/128$ at constant $\tau_f = 0.65\Delta t$. The root-mean-square values of the 2δ -discontinuity for all the four grid structures are presented in Fig. 3.7, where $\Delta x_0 = d/16$. A consistent decline in $C_{PD}^{2\delta}$ can be observed with reduction in Δx , characterized by an approximate slope of 1.67 (in a log-log plot), which is comparable to the near-quadratic decay reported by Seo and Mittal [95]. This also augurs well with the observations made using a volume-of-body IB-FV solver [82] where $C_{PD}^{2\delta} \sim \Delta x^{1.31}$, indicating that spurious force oscillations decrease at a faster than linear rate with increasing grid resolution.

The temporal force history shown in Fig. 3.8 does not have any visible spurious oscillations even on coarse meshes and has much smoother history of the pressure drag coefficient on the finest mesh. In a nutshell, the spurious force oscillations in present IB-LB framework may be related to the nodal distance as,

$$C_{PD}^{2\delta} \sim (\Delta x)^{1.67} \quad (3.7)$$

and re-emphasizes the advantage of the PSC algorithm in simulating moving boundary problems. Indeed, the subsequent section shows that this advantage of a smooth temporal history does not compromise the accuracy of the numerical solution.

A final feature of the PSC algorithm that requires exploration is the trait of volume conservation, particularly considering the continual obligation of re-defining and re-meshing the solid domain at every time-step for moving body problems, raising skepticism about possible loss of volume and accordingly affecting the overall accuracy of the simulation outcome. Referring to the cell-decomposition method illustrated in Fig. 2.2, solid sub-cells are identified based on the location of cell center with respect

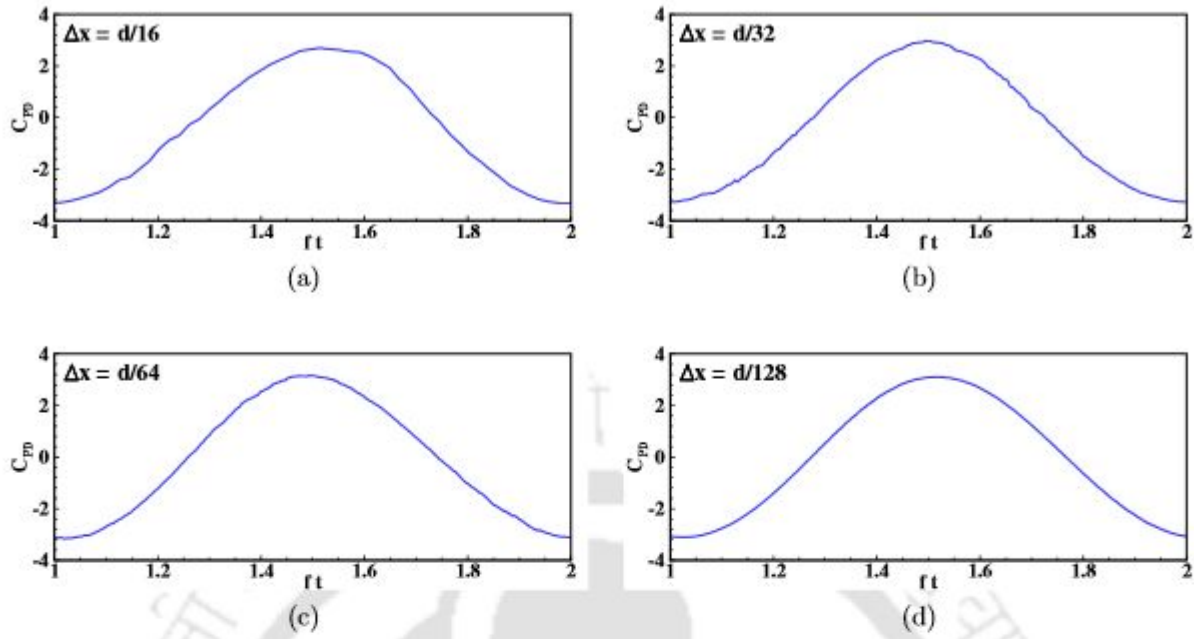


Figure 3.8: Time history of pressure drag coefficient (C_{PD}) of an inline oscillating cylinder for different grid resolution (Δx) (a) $d/16$, (b) $d/32$, (c) $d/64$ and (d) $d/128$.

to the actual solid boundary, which may introduce some volumetric error. To test this hypothesis, the temporal evolution of volumetric error for $n_{sub} = 5$ and 10 are shown in Fig. 3.9. It is clearly obvious that increasing the number of subcells decreases the volume conservation errors, albeit at a marginally increased computational cost, necessitating a trade-off. Considering the small and acceptable error levels in this problem and computational time requirement, the present work continued with $n_{sub} = 5$ for all the test cases demonstrated in the remainder of this thesis.

3.4 Numerical studies on incompressible fluid flows

The studies on accuracy, conservation and spurious force oscillations have shown that the PSC algorithm is a promising framework for further investigations. The methodology guarantees at least first-order accuracy with approximate mass conservation and leads to tolerable spurious force oscillations on moderate grid resolutions. The present section concentrates on scrutinizing its robustness and efficacy by investigating a large spectrum of test cases encompassing several stationary and moving boundary scenarios, which involves both imposed and induced motion of the particle. It must also be mentioned here that care is taken to ensure grid-independency for all the cases discussed in this section, while facilitating a trade-off between accuracy and computational cost.

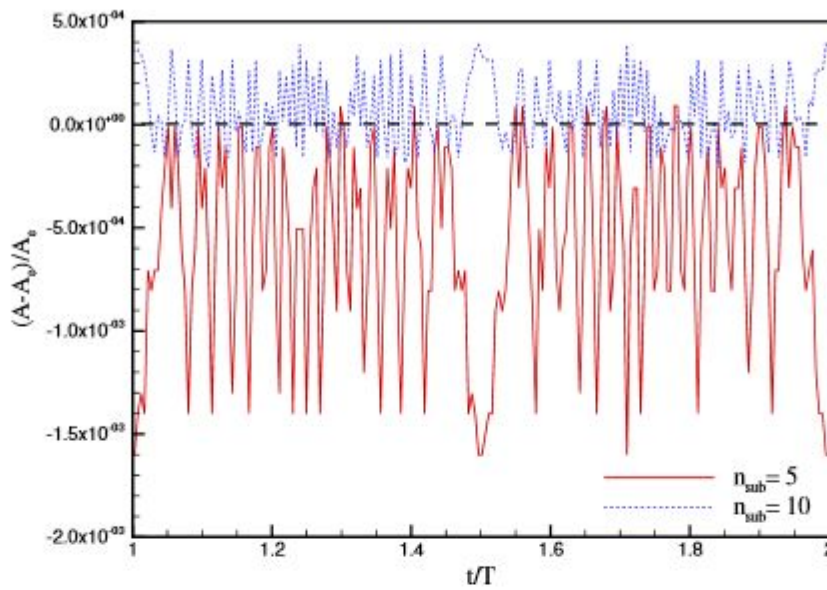


Figure 3.9: Relative volume error of the solid body over time.

3.4.1 Uniform flow past a stationary circular cylinder

The flow past a stationary circular cylinder is often viewed as a benchmark problem for hydrodynamics and also involves a non grid-aligned immobile interface. It also has direct relevance to real-life flows around bluff bodies, such as those encountered in aerodynamics, and can exhibit diverse hydrodynamics, consequently finding extensive interest in computations. The study firstly aims towards validating the solver for both steady and unsteady flows by considering a circular cylinder of diameter d placed inside a two-dimensional domain, detailed in Fig. 3.10. The computational domain is subjected to uniform flow at inlet, characterized by Re , and constant density and Neumann velocity boundary condition at exit, while the horizontal boundaries are also experiencing zero velocity gradient. The coefficient of drag (C_d) and non-dimensional recirculation length (L_r/d) rear of the cylinder for low Reynolds numbers of $Re = 20$ and 40 are presented in Table 3.3, where the data reported by several other

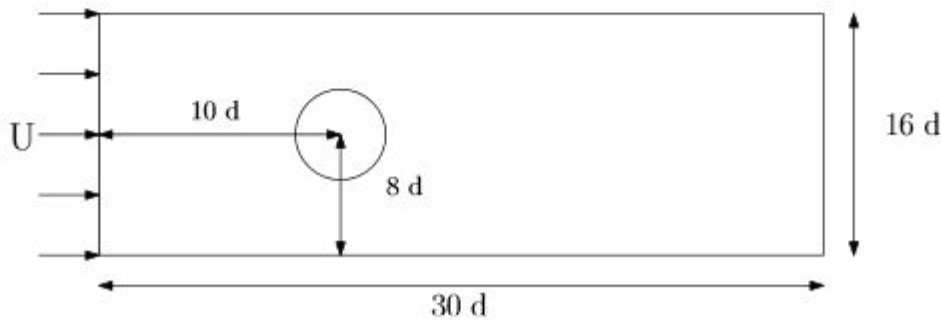


Figure 3.10: Schematic diagram of flow past a circular cylinder

Table 3.3: Comparison of coefficient of drag (C_d) and recirculation length (L_r/d) with literature.

	Method	$Re = 20$		$Re = 40$	
		C_d	L_r/d	C_d	L_r/d
Present	PSC	2.039	0.940	1.529	2.362
Dennis and Chang [96]	FDM	2.045	0.940	1.522	2.345
Ye <i>et al.</i> [97]	FVM	2.030	0.920	1.520	2.270
Wu and Shu [43]	DF-IB-LB	2.091	0.930	1.565	2.310
Kang and Hassan [98]	DF-IB-LB	2.076	0.940	1.560	2.350

researchers are also available. Numerical investigations by Dennis and Chang [96] and Ye *et al.* [97] were performed using finite difference method (FDM) and finite volume method (FVM) respectively. The results using PSC are seen to be in excellent agreement on both counts. It is also imperative to critically inspect parameters that are varying locally, such as pressure for this test case, which features a curved solid that does not conform to the underlying Cartesian mesh. The azimuthal variations in the coefficient of pressure (C_p) along the cylinder surface are compared with the results of He and Doolen [99] in Fig. 3.11. Here the pressure coefficient is defined as, $C_p = 2(p - p_{in}) / \rho_{in} U^2$, where p_{in} , ρ_{in} and U respectively represent average pressure, average fluid density and velocity at the inlet plane. It is evident from the figure that, variation of C_p is symmetrical about the central horizontal axis due to the formation

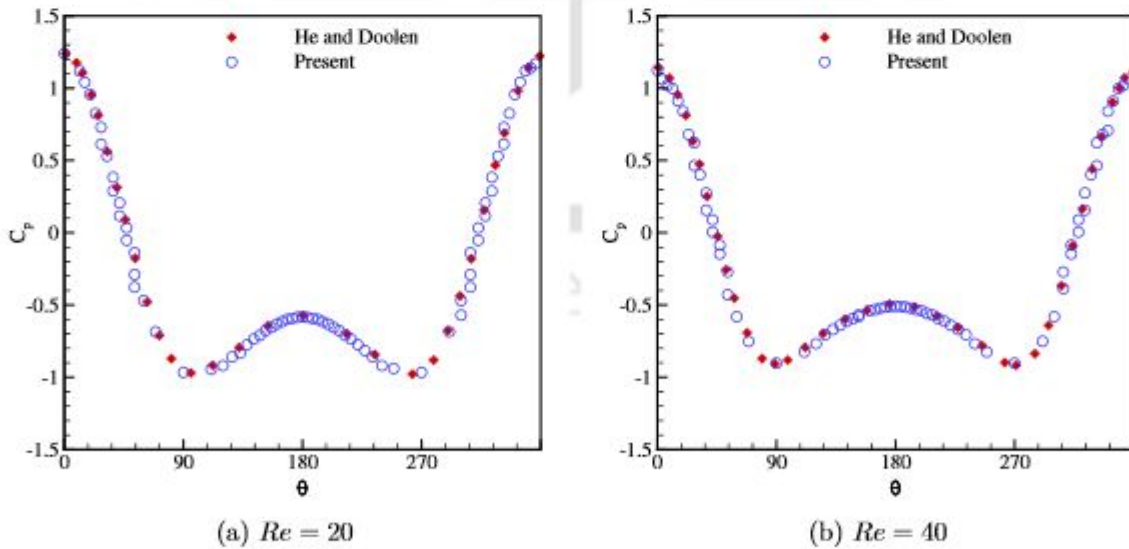


Figure 3.11: Comparison of variation of coefficient of pressure (C_p) with cylinder angle θ for (a) $Re = 20$ and (b) $Re = 40$, with He and Doolen [99]. ($\theta=0$ at stagnation point and increases along counter-clockwise direction).

Table 3.4: Comparison of average drag coefficient ($\overline{C_d}$), maximum and minimum C_l and Strouhal number (St) for different Reynolds numbers with literature for flow past circular cylinder

	Method	$\overline{C_d}$	C_l	St
$Re=100$	Present	1.368	± 0.340	0.166
	Kang and Hassan [98]	1.368	± 0.345	0.163
	Wu and Shu [43]	1.364	± 0.344	0.163
$Re=150$	Present	1.347	± 0.535	0.185
	Kang [100]	1.355	± 0.543	0.181
	Liu <i>et al.</i> [101]	1.334	± 0.530	0.182
$Re=200$	Present	1.363	± 0.706	0.197
	Braza <i>et al.</i> [102]	1.380	± 0.780	0.190
	Chen <i>et al.</i> [103]	1.374	± 0.700	0.195

of steady recirculating eddies behind the cylinder. The cylinder experiences maximum pressure at the stagnation point $\theta = 0^\circ$, whilst the lowest pressure appears around $\theta = 90^\circ$ for the cases considered here. Despite PSC being a cell-based approach, which requires the wall pressure to be evaluated at nodes in close proximity to the actual boundary and thereby raising possibility of non-smooth prediction, the present results are in excellent accord with the literature.

Further, an unsteady laminar flow is considered where initial perturbation in the flow field results in alternate shedding of vortices popularly known as Karman vortex street. The observations for three different Reynolds numbers in the shedding regime are summarized in Table 3.4, along with the selected data from literature. While the average drag coefficient ($\overline{C_d}$) remains nearly unchanged with increase in Re , the lift coefficient (C_l) and Strouhal number ($St = f^d/\nu$) exhibit gradual increase but all quantities agree well with those reported in open literature. Time histories of both drag and lift coefficients are also presented in Fig. 3.12. Beyond a period of initial development, drag coefficient shows very little fluctuations, adhering the mean value quite closely. The lift coefficient, however, experiences fluctuations with much larger amplitude, albeit following a periodic pattern with a periodicity twice that of the drag coefficient. Fig. 3.13 presents the steady-state vorticity contour for a low- Re flow, characterized by symmetrical recirculation zones, and the instantaneous contours for a moderate- Re flow, displaying the unsteady Karman vortex street.

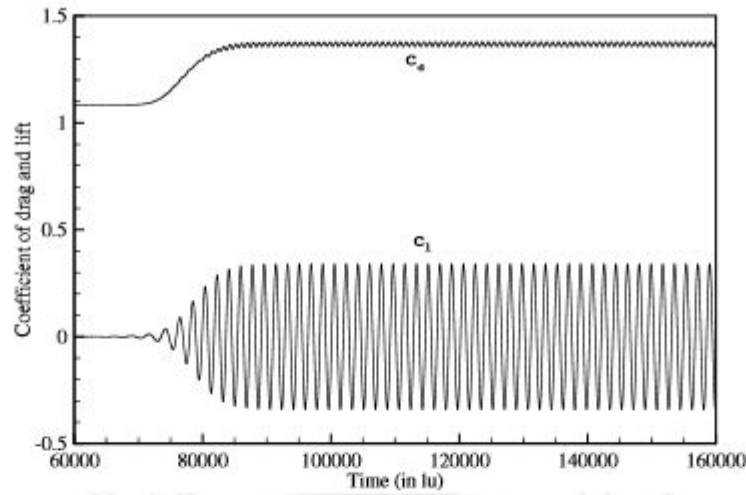
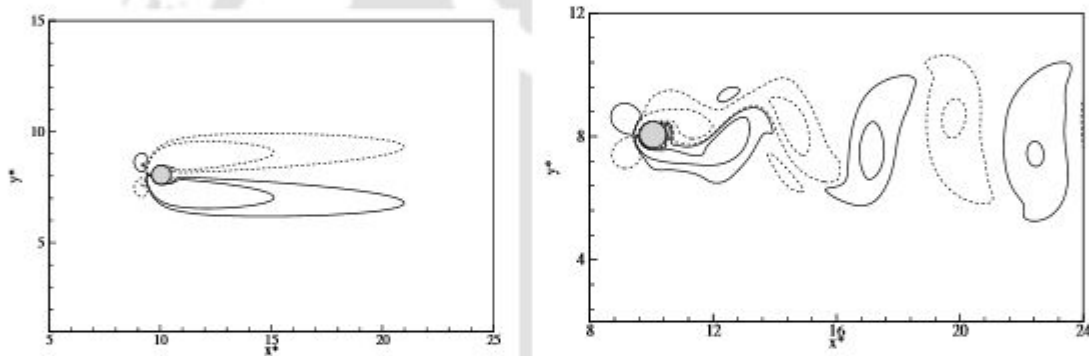


Figure 3.12: Temporal history of drag and lift coefficients for flow past stationary circular cylinder at $Re = 100$.



(a) Vorticity contour behind the cylinder at $Re = 20$ (b) Instantaneous vorticity contour behind the cylinder at $Re = 100$

Figure 3.13: Vorticity contours behind the cylinder (solid and dashed lines represent positive and negative vorticity respectively).

3.4.2 Flow induced by inline oscillating cylinder

Having validated the PSC algorithm for a problem involving stationary body, moving body problems with enforced motion are now considered. As a first moving body test, a circular cylinder of diameter d is placed at the middle of a quiescent fluid domain of size $30d \times 20d$ (Fig. 3.14) which is subjected to a harmonic oscillation of the following form.

$$X_c = X_{c0} - A \sin(2\pi ft) \quad (3.8)$$

where the used notations have similar meanings to those in Eq. (3.3). The periodic movement of the cylinder triggers fluid motion and the unsteady hydrodynamics can

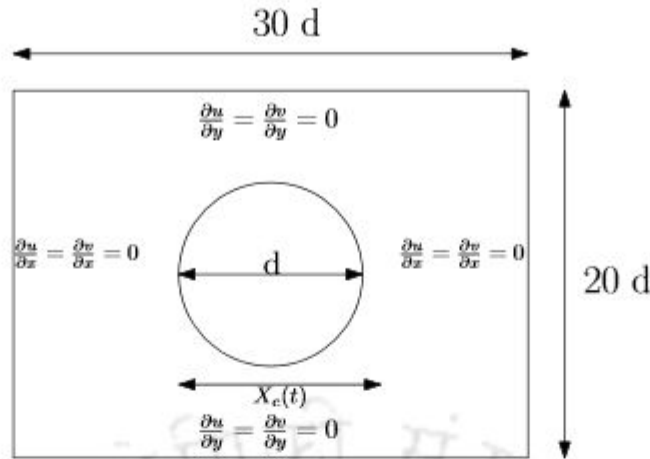


Figure 3.14: Schematic of oscillating cylinder immersed into an enclosure

be characterized in terms of Reynolds number ($Re = U_0 d / \nu_f$) and Keulegan-Carpenter number ($KC = U_0 / f d$), with U_0 being the maximum velocity. A constant value of $KC = 5$ is maintained, while studies have been performed for Re values of 10 and 100. Neumann boundary condition is realized at all the four domain boundaries, whereas the cylinder surface is a no-slip wall.

Vorticity contours, velocity vectors and streamlines in the vicinity of the cylinder for different phase angles of cylinder oscillation are shown in Fig. 3.15 and 3.16 for $Re = 100$. It can be observed that an upper and lower boundary layer flow is developed in front of the cylinder during its forward motion. As a result of flow separation, two counter-rotating vortices of same strength and shape are developed. Owing to the backward motion of the cylinder (after half a cycle), the vortex pair produced during forward motion starts splitting resulting in a wake reversal. The comparison of the velocity profiles in the vicinity of the cylinder for different phase angles with the experimental data of Dütsch et al. [104] at four different locations exhibit fairly consistent match, in terms of both magnitude and silhouette.

A pertinent aspect of study in this test problem pertains to the accuracy of the

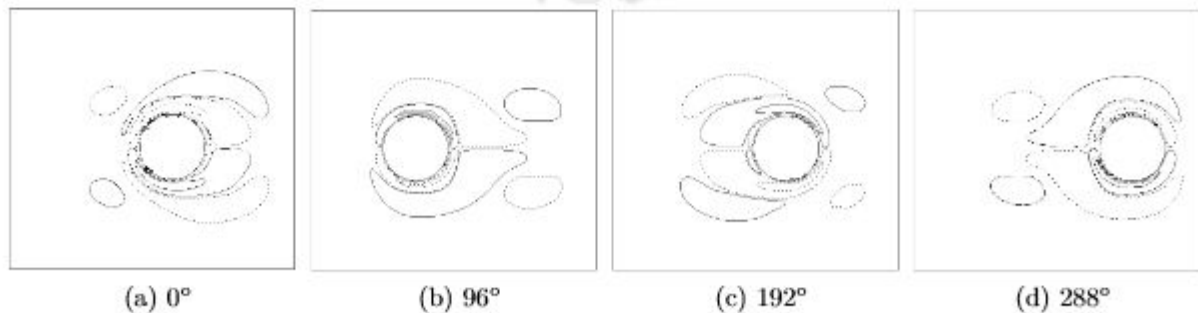


Figure 3.15: Vorticity isolines at different phase angles for $Re = 100$ and $KC = 5$ (solid and dashed lines represent positive and negative vorticity respectively).

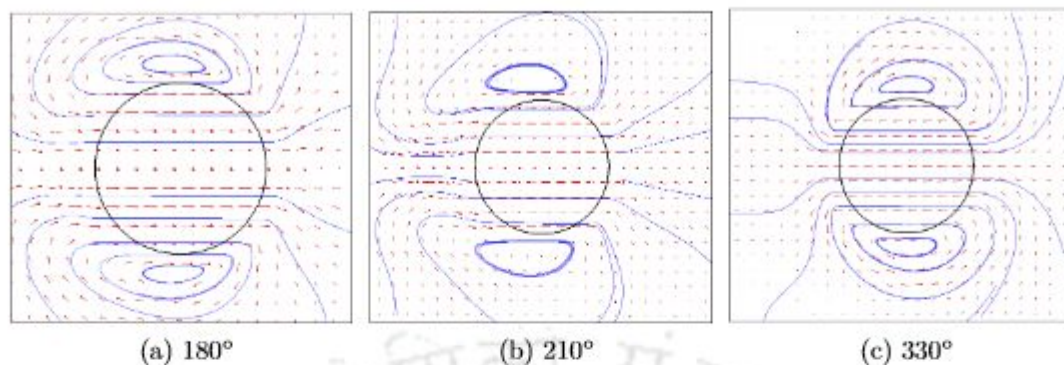
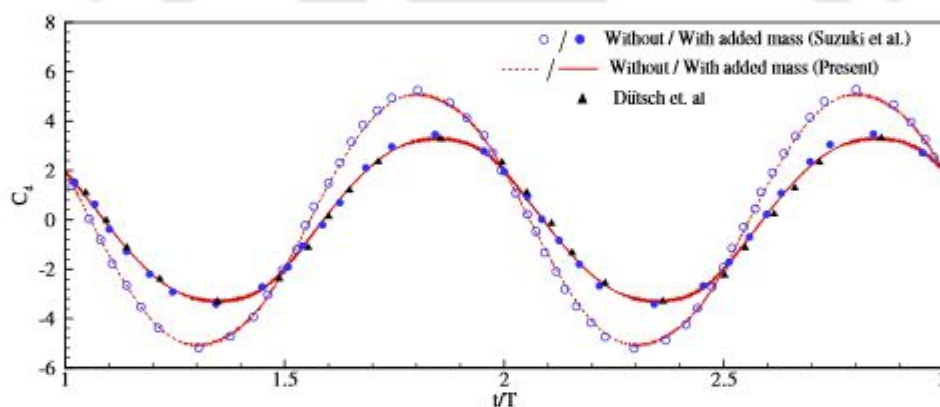
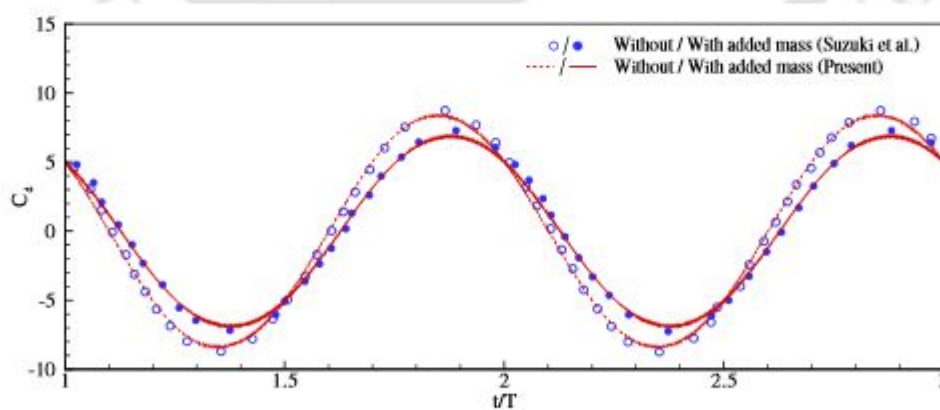


Figure 3.16: Velocity vectors and streamlines in the vicinity of cylinder different phase angles for $Re = 100$ and $KC = 5$.



(a) $Re = 100$ and $KC = 5$



(b) $Re = 10$ and $KC = 5$

Figure 3.17: Comparison of variation of coefficient of drag C_d with respect to time cycle between PSC and Dütsch et al. [104] and Suzuki and Inamuro [91] at $KC = 5$ and (a) $Re = 100$ and (b) $Re = 10$.

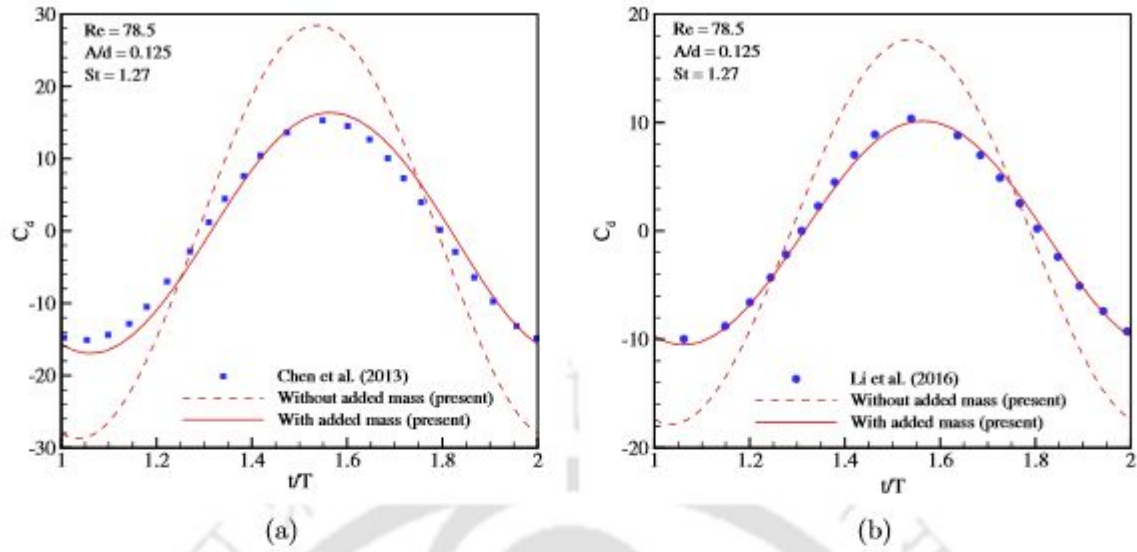


Figure 3.18: Comparison of coefficient of drag of PSC with (a) Chen et al. [47] and (b) Li et al. [105] at $Re = 78.5$, $A/d = 0.125$ and $St = 1.27$

time history of force coefficients. Figure 3.17 indicates that the stream-wise drag coefficients from the PSC approach compare well with earlier computations and experimental data. The excellent comparison is however possible for a higher Re only when the added mass term is accounted for. A higher Reynolds number corresponds to greater particle acceleration and neglecting the added mass term leads to inaccurate peak amplitude of the drag coefficient although there are no perceptible phase errors as is evident from Fig. 3.18. It must be remarked that the need for considering added mass effect for accelerating bodies has however found no mention in earlier works adopting LB methodology, regardless of following PSC [47] or bounce-back schemes [105].

The comparison in Fig. 3.19 further highlights the considerable suppression of spurious force oscillations in this case. Evidently, the amplitude of spurious oscillations from the PSC approach is significantly smaller when compared to those from conventional sharp-interface IB approaches [95, 100, 106]. This attribute of the PSC approach also closely mirrors the diffuse interface immersed boundary/finite volume method [81, 82] which also employs a solid-fraction based unified evolution equation for the macroscopic variables. It must be mentioned that Kang [100] reported severe spurious oscillations with sharp-interface IB-LB schemes which may be mitigated by using standard smoothing or FFT filtering techniques, at the cost of additional computation. He also adopted the concept of effective radius in direct-forcing IB-LB scheme to abate over-prediction of surface force coefficients. In contrast, the PSC methodology requires no such ancillary treatment for accurate prediction of interfacial physics

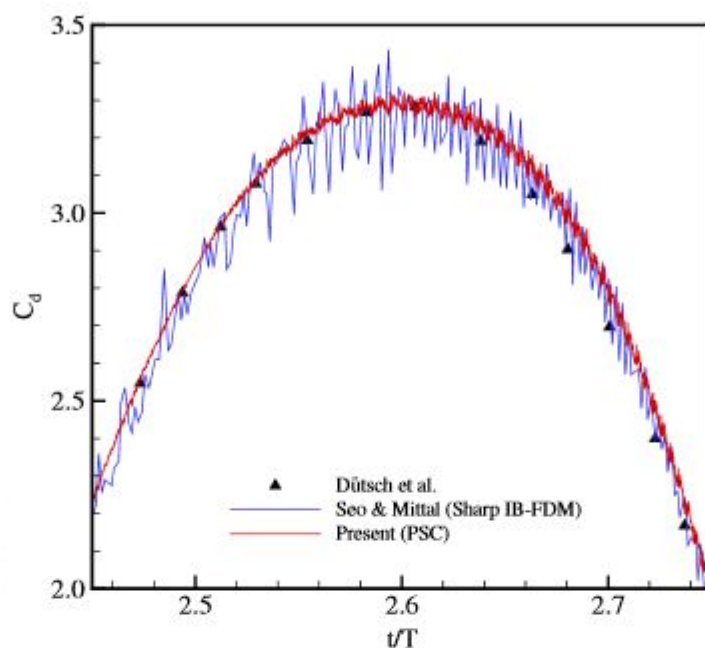


Figure 3.19: Comparison of spurious fluctuations in coefficient of drag C_d between PSC and Seo and Mittal [95] for $Re = 100$ and $KC = 5$.

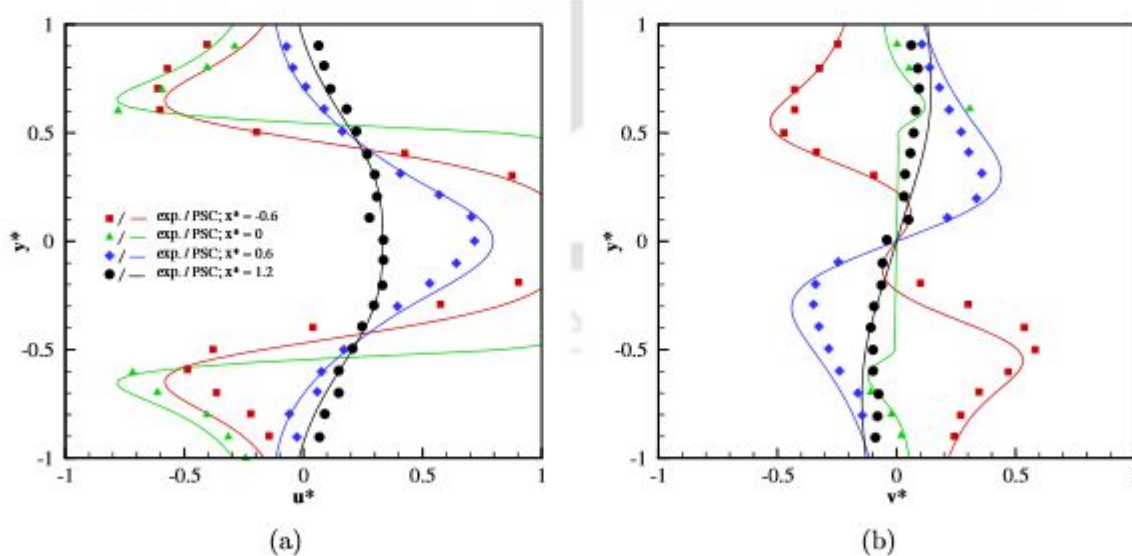


Figure 3.20: Comparison of velocity profiles between PSC and experimental data obtained by Dütsch et al. [104] at phase angle 180° for $Re = 100$ and $KC = 5$. x^* and u^* represents non-dimensionalized position and velocity respectively.

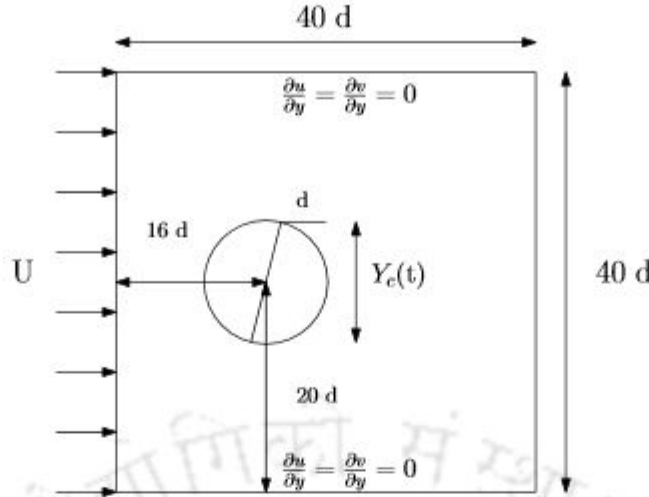


Figure 3.21: Schematic of oscillating cylinder immersed into an enclosure having uniform velocity inlet

and unlike cut-cell based sharp-interface IB approaches [47, 95] has a simple implementation that approximately conserves geometrical volume and results in acceptably accurate numerical solutions. Furthermore, Fig. 3.20 reveals computed horizontal and vertical velocities using PSC are in good agreement with experimental data obtained by Dütsch *et al.* [104].

3.4.3 Flow past a transverse oscillating cylinder

In order to further test the PSC methodology for fluid-particle interaction problems with moving bodies, an imposed transverse oscillation of a cylinder in a flow field is considered. This test case considers a non-quiescent flow with a prescribed velocity inlet and to the best of author's knowledge has not been simulated using PSC approach till date, despite the involvement of intricate hydrodynamics. In this study, a circular cylinder of diameter d is immersed in a flow field of dimension $40d \times 40d$ (Fig. 3.21). A uniform velocity field corresponding to Reynolds number 185 is invoked at the inlet and constant pressure is satisfied at the outlet. Neumann boundary condition with zero velocity gradient is applied at top and bottom sides of the computational domain and no-slip condition is satisfied on the cylinder surface. The forced motion of the cylinder follows a periodic pattern given as,

$$Y_c(t) = Y_{c0} - A \sin(2\pi f_e t) \quad (3.9)$$

with Y_c , Y_{c0} , A and f_e representing instantaneous vertical position of the cylinder centre, initial position of the same at $t = 0$, enforced amplitude of oscillation ($= 0.2d$) and excitation frequency respectively.

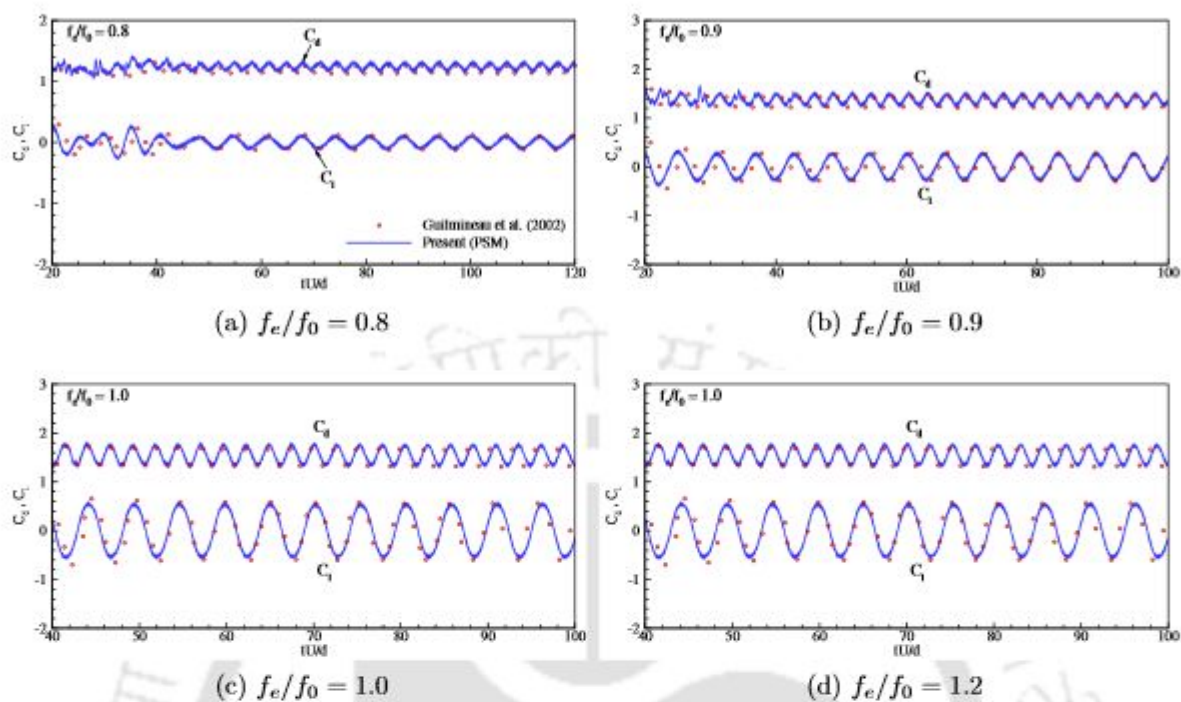


Figure 3.22: Variation of coefficient of drag C_d and lift C_l with respect to time cycle at different frequency ratio and its comparison with Guilmineau and Queutey [107]

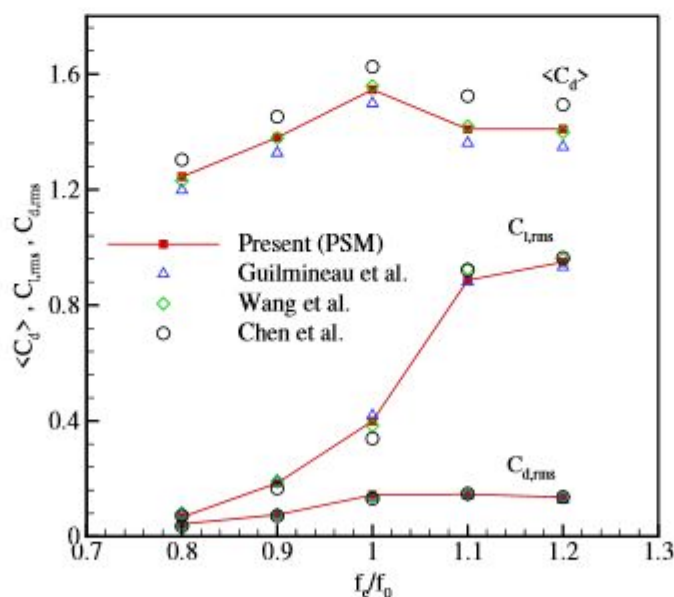


Figure 3.23: Comparison of flow coefficients for flow past a transverse oscillating cylinder using PSC with the literature.[103, 107, 108]

Simulations are performed for several values of the frequency ratio $f = f_e/f_0$. Here, f_0 is the natural vortex shedding frequency corresponding to Strouhal number (St) of 0.192, which is obtained beforehand by simulating flow past a stationary circular cylinder at $Re = 185$. It can be observed from time histories of the coefficient of drag and lift (Fig. 3.22) that spurious force oscillations are not prominent in the present study and results obtained are in good agreement with literature. Figure 3.23 shows the comparison of time-averaged coefficient of drag ($\langle C_d \rangle$), RMS coefficient of drag and RMS coefficient of lift obtained using PSC approach with those reported in open literature [103, 107, 108].

3.4.4 Flow past a rotating circular cylinder

Having considered translational imposed motions, flow past a rotating circular cylinder is now considered, which is also a test problem not simulated using PSC till date. The cylinder is assumed to be rotating with a constant angular velocity, thereby eliminating any rotational acceleration of the solid. A uniform velocity field corresponding to Reynolds number of 100 is invoked at the inlet and constant pressure is set at the outlet. Neumann boundary condition is applied at top and bottom faces of the computational domain, while non-slip condition is satisfied on the cylinder surface. The geometrical details are shown in Fig. 3.24. Forty nodes along the diameter of the cylinder suffice for the simulations with non-dimensional rotation rates ($\alpha = 0.5d\Omega_P/U$) of 1.0. A comparison of the present results using PSC approach are compared with literature in Table 3.5. Computed values of the average drag ($\bar{C}_d$) and lift coefficient ($\bar{C}_l$) and Strouhal number (St) are in reasonable agreement with literatures studied herein. It must be remarked that unlike the translational cases, the added mass term, although

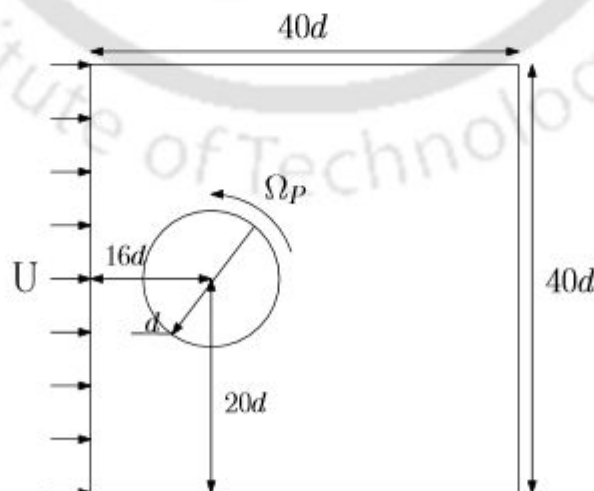


Figure 3.24: Schematic of rotating cylinder immersed into an enclosure having uniform velocity inlet

Table 3.5: Comparison of average drag coefficient ($\overline{C_d}$), average lift coefficient ($\overline{C_l}$) and Strouhal number (St) for $Re = 100, \alpha = 1.0$ with literature for flow past rotating circular cylinder.

$Re = 100, \alpha = 1.0$	$\overline{C_d}$	$\overline{C_l}$	St
PSC	1.172	-2.412	0.166
Kang et al. [109]	1.040	-2.488	0.166
Stojković et al. [110]	1.108	-2.504	0.166
Paramane and Sharma [111]	1.095	-2.490	0.165

included herein, has no effect for this test case since there is no rotational acceleration. Moreover, there are no fresh/dead cells because of the motion and no spurious force oscillations are observed in this study.

3.4.5 Sedimentation of a symmetrically placed particle

Having explored the ability of PSC approach to simulate linear and rotational imposed motion, the PSC methodology is now subjected to fluid-particle interaction problems involving particle motion induced by gravity. Firstly, the numerical experiment of sedimentation of a circular particle is performed in a narrow quiescent medium whose computational domain, material properties and boundary conditions are set according to Glowinski et al. [112]. In Fig. 3.25, the dimensions are set as, d (diameter of particle) = 0.25 cm, $a = 1$ cm, $H = 6$ cm, $L = 2$ cm, $h = 4$ cm and g represents acceleration due to gravity. Initially both fluid and particle are at rest, the position of the particle at $t = 0$ being marked in the figure. The density (ρ_f) and dynamic

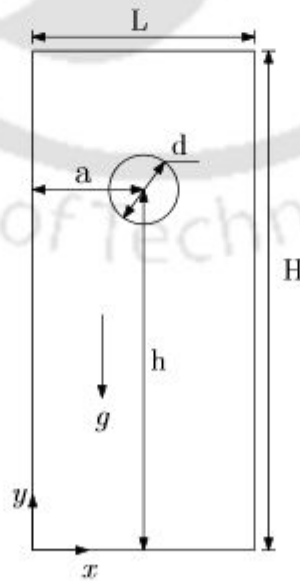


Figure 3.25: Schematic of sedimentation of a particle

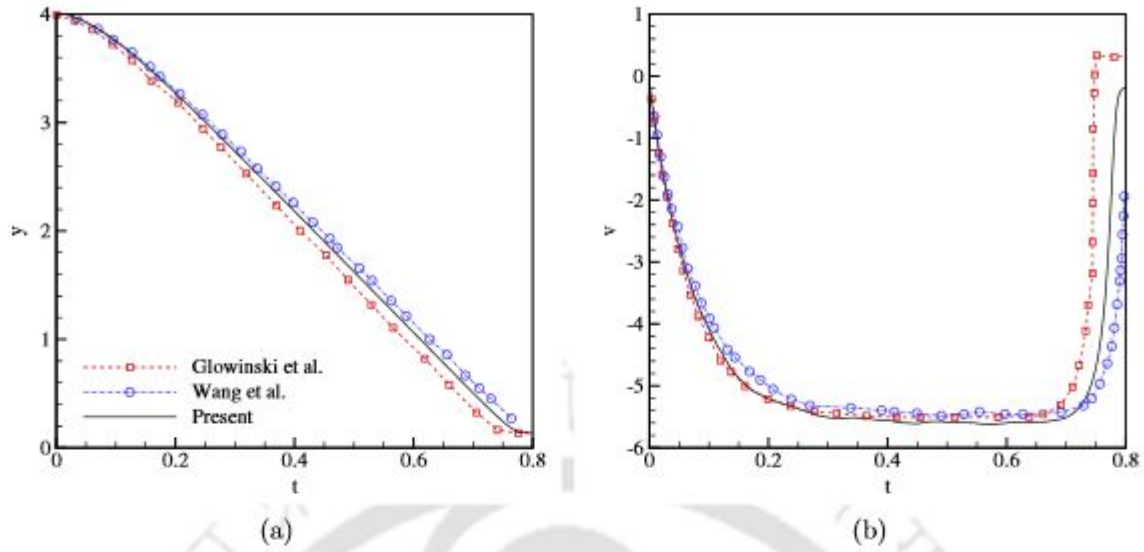


Figure 3.26: Time evolution comparison of (a) longitudinal coordinate of the particle and (b) longitudinal velocity of the particle while freely falling in an enclosure literature. [108, 112]

viscosity (μ_f) of the fluid are selected as 1 g/cm^3 and 0.1 g/cm s respectively, while the particle is 1.25 times denser than the fluid. Forty nodes are placed along the diameter of the cylinder and relaxation time is set as $\tau_f = 0.8$ during the present simulation where the cylinder has three degrees of freedom.

The variation of position and velocity of this circular particle in the y -direction, which is positive downwards, with time are compared with reported results in literature in Fig. 3.26. The present solver's data agree well with the results obtained with a Lagrange-multiplier based fictitious domain approach by Glowinski et al. [112] as well as the IB-LB solver based on fractional step method proposed by Wang et al. [108]. Glowinski et al. [112] reported that the particle moves slightly towards right of the axis of vertical symmetry of the enclosure in the course of its journey. This symmetry-breaking was attributed to the triggering of perturbations associated with the selection of their numerical procedure. No such symmetry-breaking nor appearance of rotational kinetic energy is observed using PSC. Time histories of the particle's Reynolds number (Re_P) and translational kinetic energy (E_t) are also compared with literature [108, 113] in Fig. 3.27 where the quantities are defined as,

$$E_t = 0.5m_p (\mathbf{u}_c^2 + \mathbf{v}_c^2), \quad Re_P = \frac{\sqrt{\mathbf{u}_c^2 + \mathbf{v}_c^2} d}{\nu_f} \quad (3.10)$$

Here, m_p and I_p are mass and mass moment of inertia of the particle. The maximum particle Reynolds number Re_P using PSC approach is found to be 17.57, which is in

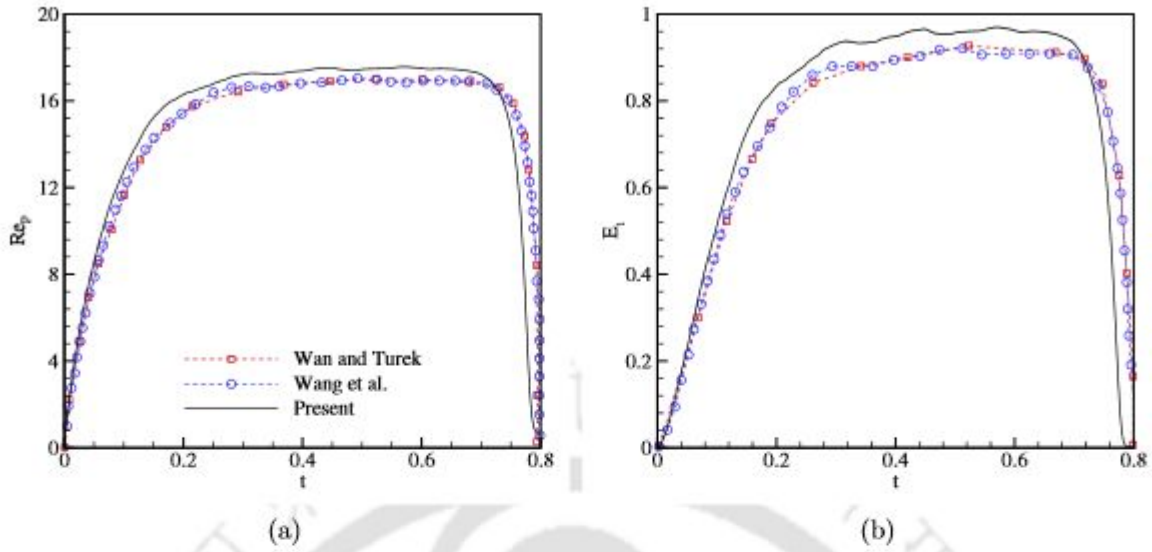


Figure 3.27: Time evolution comparison of (a) particle Reynolds number and (b) translational kinetic energy of the particle with literature. [108, 113]

well agreement with the value of 17.51 reported by Glowinski et al. [112]. Figure 3.28 shows the time evolution of vorticity contours while the particle is freely falling in the enclosure, which also indicates that the particle falls vertically and attains the terminal velocity well before it strikes the bottom of the enclosure.

3.4.6 Sedimentation of an asymmetrically placed particle

The symmetric nature of the previous configuration resulted in solely one-dimensional translational motion of the particle, as can be substantiated by near-zero magnitudes of the x -component of velocity and angular acceleration. To evaluate the PSC methodology for a genuinely three degree-of-freedom case, the previous arrangement is modified to orient the initial location of the particle away from the centerline. The repelling effect inflicted by the boundary layer developed on the nearer wall is expected to shove the particle towards the center and, with gravity acting vertically downward (positive y -direction), induce angular acceleration.

The computational domain and boundary conditions are selected according to Wen et al. [114]. Following the schematic in Fig. 3.25, dimensions are set as $d = 0.1$ cm, $L = 0.4$ cm and $a = 0.076$ cm. The height (H) of the enclosure can be taken such that adequate physics is captured till the particle settles at the bottom. Stipulated values of concerned particle-to-fluid density ratio (ρ_p/ρ_f) and fluid kinematic viscosity (ν_f) are 1.01 and 0.01 cm²/s respectively. In the present simulation, 26 nodes along the cylinder's diameter is considered at the LB-level, which leads to the domain being discretized into 104×800 lattice nodes. This corresponds to a physical grid

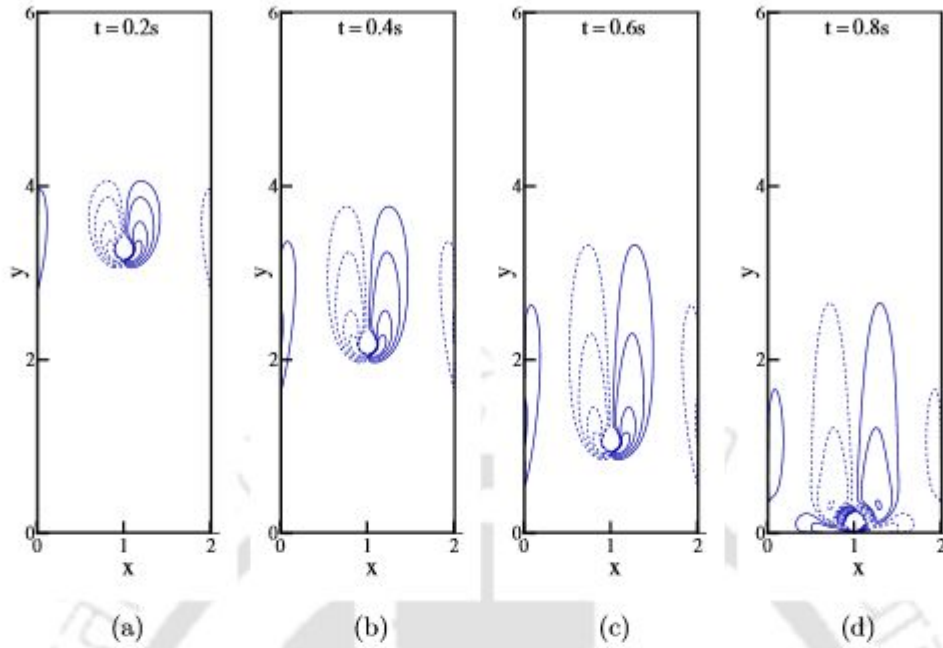


Figure 3.28: Time evolution of instantaneous vorticity contours of a symmetrically placed particle sedimentation

resolution of $\Delta x = 3.85 \times 10^{-3}$ cm and time step size, $\Delta t = 4.93 \times 10^{-5}$ s. The particle descends through the fluid adopting a circuitous orbit and its trajectory is governed by the Newtonian dynamics, which necessitates an interplay among the gravitational, inertial and viscous forces within the fluid domain. The particle trajectory and time history of relevant velocity components can be inferred from the plots presented in Fig. 3.29 and 3.30 respectively. Once the particle is allowed to descend under the action of gravity, it experiences a brief period of quivering, before settling along the centroidal axis around $t = 2$ s, and subsequently continuing with a near-constant vertical velocity till it reaches the base of the enclosure. No wall collision model is included here, as it is extraneous to the scope of the present study. Despite the absence of a particle-wall collision model, the hydrodynamics is complex and the PSC methodology is able to reproduce the same with excellent accuracy, as can be corroborated by comparing with the trends reported by Wen et al. [114]. The magnitude of terminal Reynolds number predicted by the present solver is 3.37, which is in close proximity to the value of 3.23 documented by Wen et al. [114].

3.4.7 Sedimentation of two particles of different weight

The final demonstration of the proficiency of the PSC methodology in replicating complex phenomena in fluid-particle interactions is a two-particle sedimentation problem. Two circular cylinders of identical dimension, but unequal densities are allowed to fall

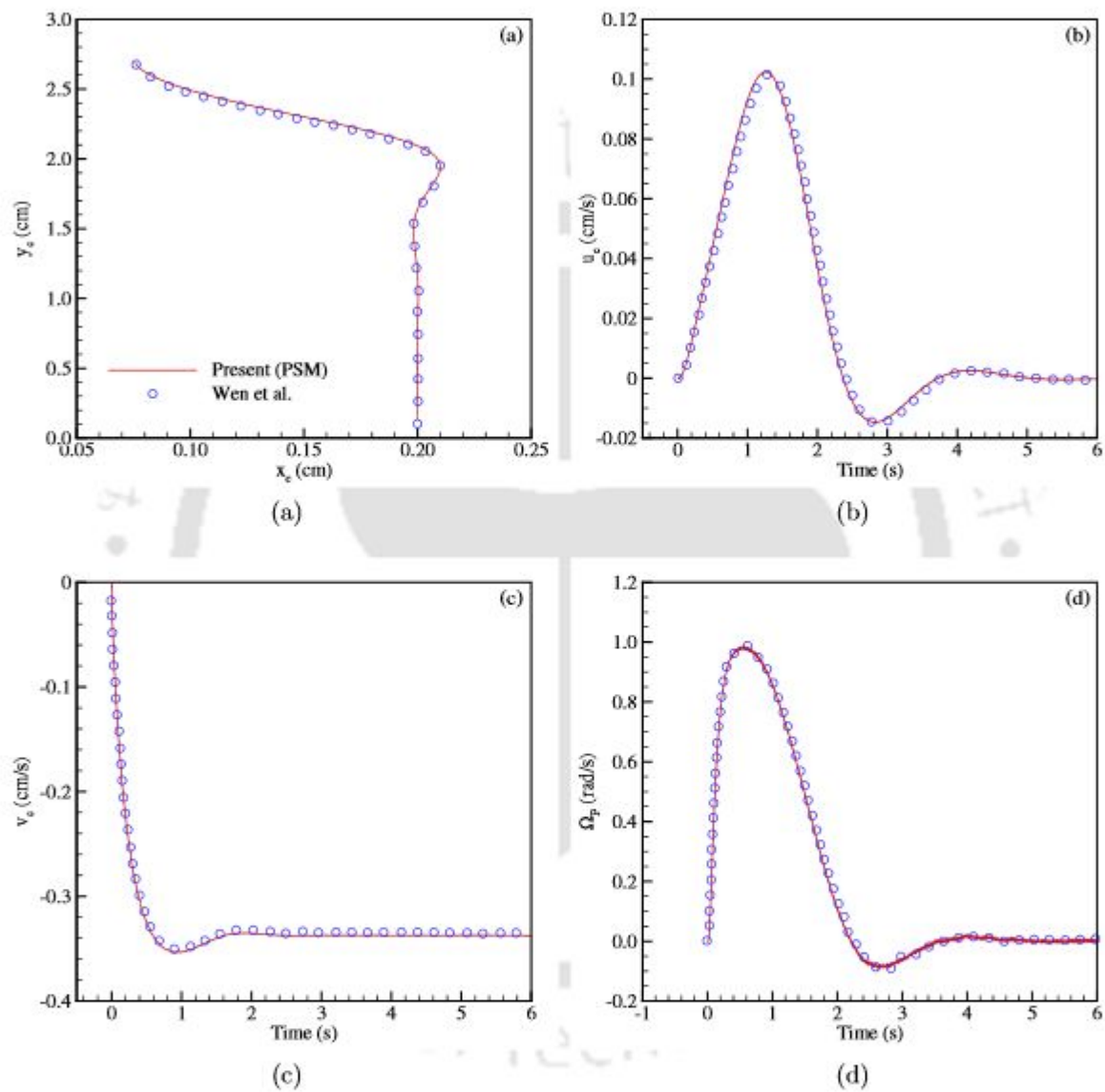


Figure 3.29: Comparison of (a) Trajectory of the particle, time dependent history of (b) velocity in horizontal direction, (c) velocity in vertical direction, (d) angular velocity of particle with Wen et al. [114].

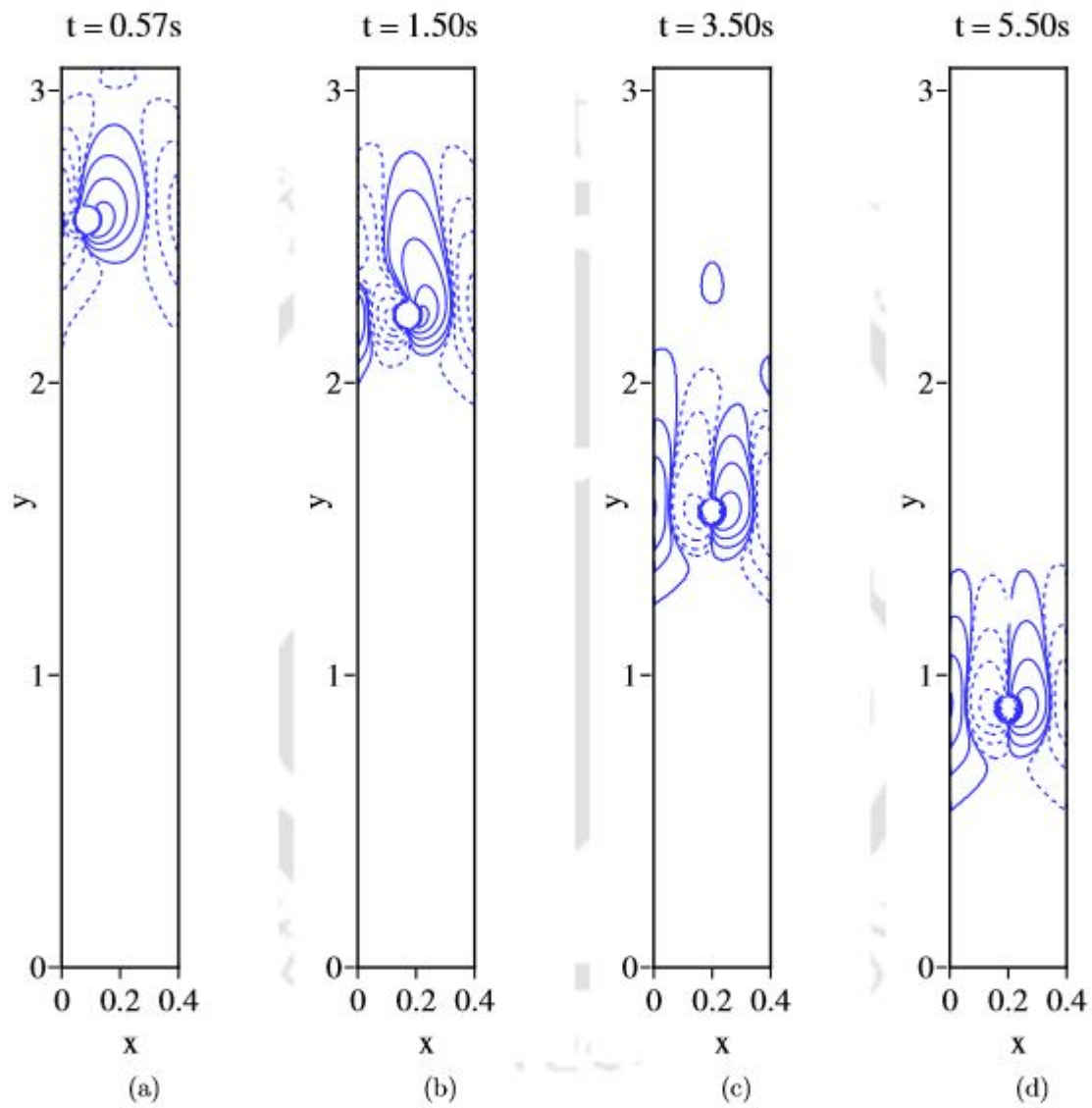


Figure 3.30: Time evolution of instantaneous vorticity contours of a asymmetrically placed particle sedimentation

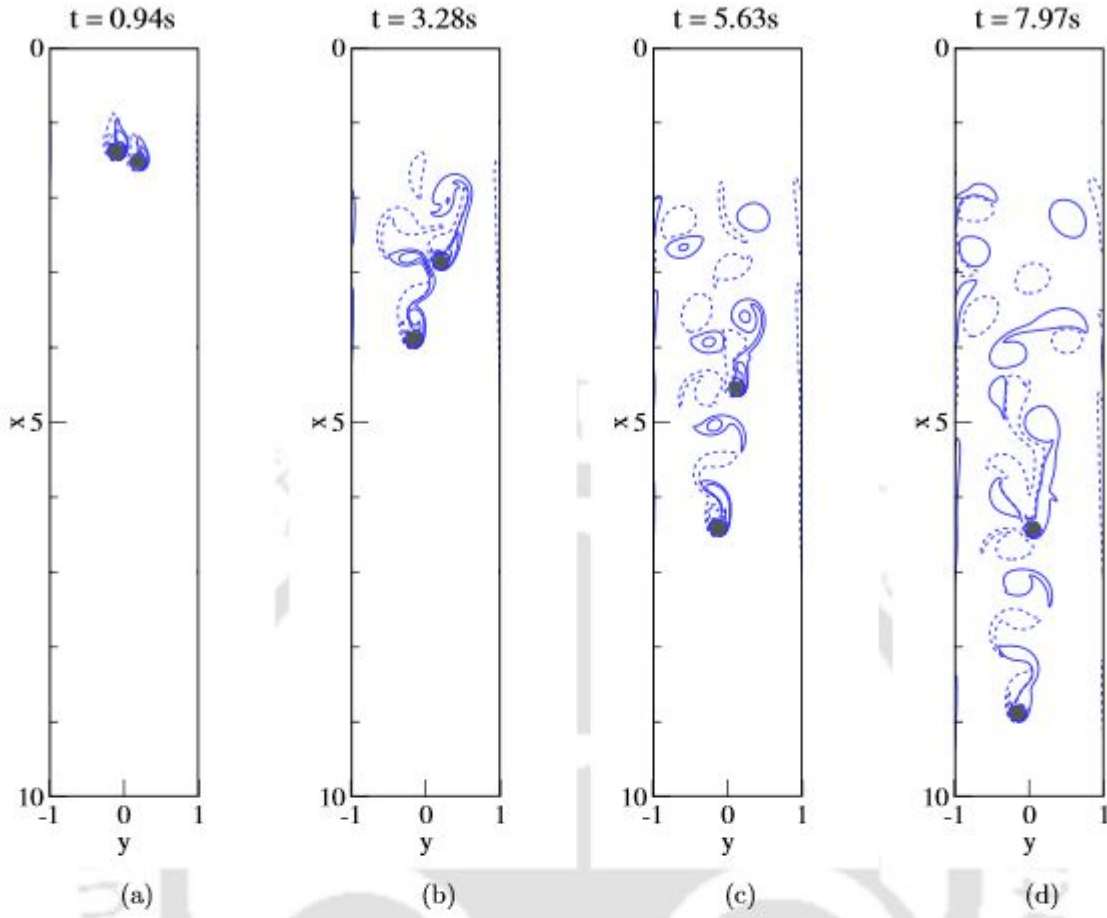


Figure 3.31: Time evolution of instantaneous vorticity contours of two particle sedimentation

freely under gravity within a quiescent fluid column. Once they are suitably positioned at the instant of inception, the trailing particle can be expected to encroach into the wake developed at the rear of the leading particle, raising the prospect of fascinating hydrodynamic communications. Such an event is more likely with the heavier particle being the leading one, as it is expected to descend faster owing to the larger mass. Therefore such a computational effort embraces multi-faceted force interaction for each particle, with the reduced-pressure region interior to the wake adding a new dimension towards dictating the motion of the trailing particle.

The investigation considers two particles of diameter $d = 0.2$ unit, which are initially located at $\mathbf{X}_c^{(1)}|_{t=0} = (0.8, -0.13)$ and $\mathbf{X}_c^{(2)}|_{t=0} = (1.2, 0.13)$ respectively in a rectangular domain of size $[0, 10] \times [-1, 1]$. Particle-to-fluid density ratios are selected to be similar to the work of Uhlmann [89] as $\rho_p^{(1)}/\rho_f = 1.5$ and $\rho_p^{(2)}/\rho_f = 1.25$. Kinematic viscosity of the fluid is set to be 8×10^{-4} units. A discrete domain of size 4000×800 is adopted with $\Delta x = \Delta y = 0.0025$ unit and $\tau_f = 0.59$, which corresponds to a physical time step of 2.344×10^{-4} s. These numbers can be combined to yield

a lattice-level gravity of 2.156×10^{-4} lattice-units. Simulations are carried out with zero velocity initialization everywhere within the domain and continued till a physical time of 8.648 s, which corresponds to the heavier particle reaching within $2d$ distance from the base of the domain. The predicted maximum particle Reynolds numbers with the PSC approach of both particles are 279.08 and 237.47, which are very close to the one obtained by Uhlmann [89] (280 and 230 respectively). Figure 3.31 shows instantaneous vorticity contours of two particles at different time levels illustrating the complex induced motion of the particles. One can also observe from Fig. 3.32a that the heavier particle exhibits an undulated trajectory as compared to the lighter particle due to oscillating lift force produced by its vortex shedding while the latter one exhibits deviation from vertical trajectory because of its presence and interaction with the preceding vortices. Moreover, Fig. 3.32e reveals that the heavier particle reaches maximum velocity at an early stage and decelerates when it enters a steady periodic vortex shedding state. The strong interaction of the trailing lighter particle with the vortices is also evident from Fig. 3.32f which reveals an increase in its angular velocity with time while the heavier particle has negligible angular velocity. Furthermore, the data obtained in Fig. 3.32 using PSC are in excellent agreement with the same reported by Uhlmann [89]. The ability of the PSC approach in accurately resolving the complex dynamics of a multi-body problem is sufficient proof that the present approach offers an excellent alternative to conventional N-S solvers for accurate computation of incompressible fluid-structure interaction problems.

3.5 Summary

The present chapter demonstrates a comprehensive evaluation of the Partially Saturated Computational cells (PSC) approach for incompressible hydrodynamics involving one or more rigid bodies undergoing imposed and induced motion. Studies on accuracy with the PSC approach reveal that it is nominally second-order accurate with errors smaller for values of relaxation time $\tau_f < 1$. For moving boundary problems though the spatial accuracy in velocity prediction declines towards first-order owing to the diffuse nature of the interface. The solid collision operator is found to be strongly influenced by the choice of τ_f . But for stable computations with $\tau_f < 1$, the PSC approach exhibits negligible compressibility errors and a mass defect that reduces with increasing grid resolution. The PSC approach also leads to much lesser spurious force oscillations (SFOs) for moving body problems on a given lattice and the oscillations reduce super-linearly with grid refinement. The studies on SFOs and discrete mass conservation of the PSC approach are novel aspects of the present study that have not been dealt with in past studies. A wide range of problems that range from flow

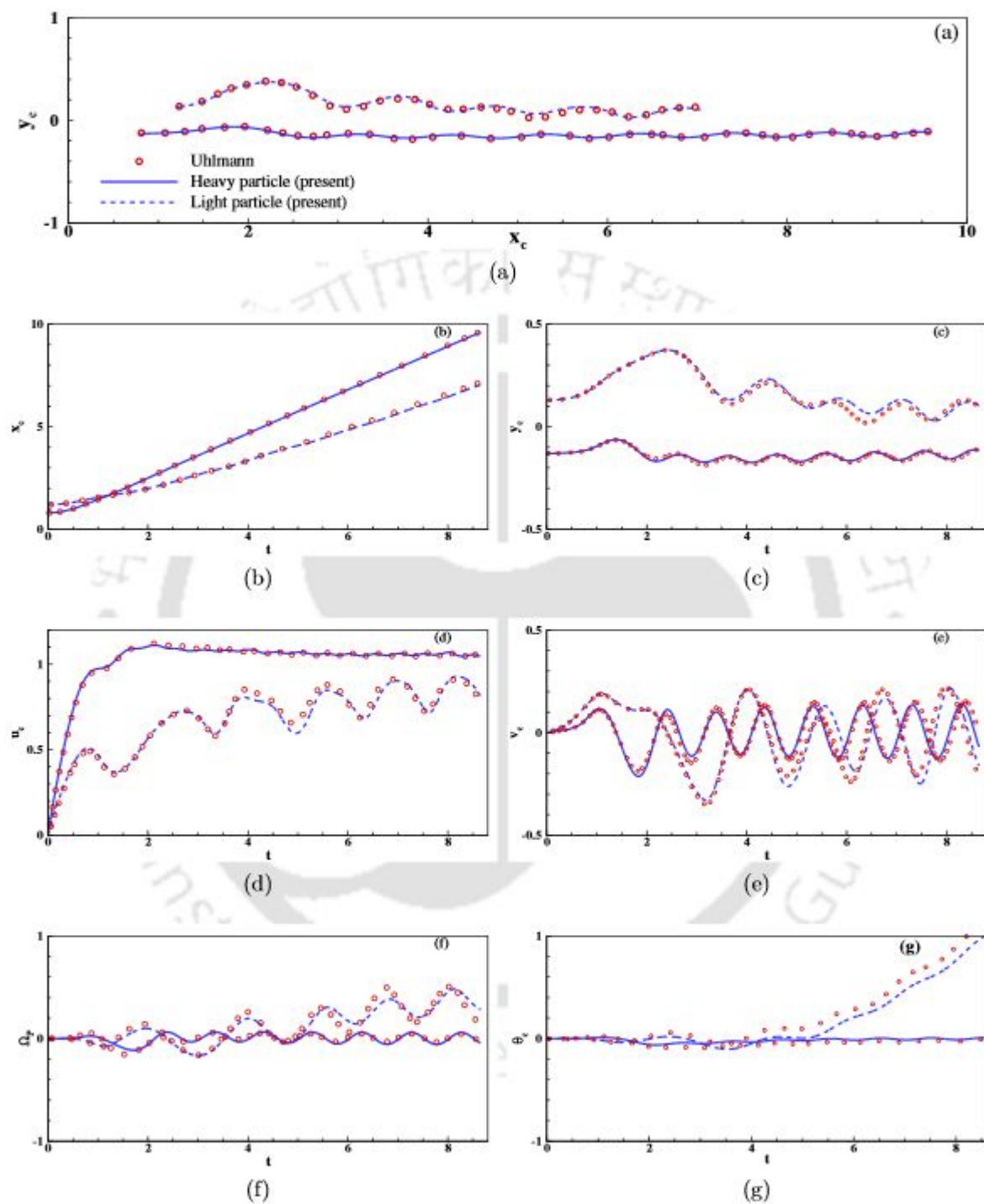


Figure 3.32: Sedimentation of particles of different weight (a) trajectory, time evolution of particles' (b-c) center location, (d-e) linear velocities, (f) angular velocity and (g) angular location.

past a stationary cylinder to two-particle sedimentation showcase the ability of the PSC approach in accurately computing the flow dynamics, whilst also highlighting the importance of accounting added mass effects for higher Reynolds number flows. The sensitivity of the relaxation time and the difficulty in handling Neumann boundary conditions need further exploration. The present work, which supplements the recent studies of Rettinger and Rde [50] and those of Haussmann and co-workers [51], clearly highlights that the PSC approach is a promising alternative for incompressible hydrodynamics and it is extended to solve fundamental problems and engineering applications involving heat transfer in the subsequent chapters.



CHAPTER 4

PARTIALLY SATURATED CELLS METHOD FOR THERMAL FLOWS

“Debugging is twice as hard as writing the code in the first place. Therefore, if you write the code as cleverly as possible, you are, by definition, not smart enough to debug it”

- Brian Kernighan, *Kernighan’s Law*

This chapter presents a comprehensive investigation of Partially-Saturated-Cells method (PSC) for the simulations of incompressible thermal flows in this chapter. The focal points of the investigation comprise the evaluation of its order of accuracy, Galilean invariance and efficacy to simulate heat transfer processes. The analysis reveals that the method is first-order accurate for moving body simulations irrespective of the straight or curved boundary. It is also Galilean invariant and demonstrates identical heat transfer characteristics in stationary and moving reference frames. In addition to it, a thorough analysis of the PSC algorithm is presented to enlighten its suitability for predicting thermo-hydrodynamic characteristics in free, forced, and mixed convection phenomena involving both stationary and moving boundary scenarios. So far these aspects pertaining to the thermal-PSC methodology have not been discussed in the literature to the best of author’s knowledge.

The thermal-PSC methodology introduced in Chapter 2 identifies itself as a diffuse-interface immersed boundary method; however, it differs from the conventional IB-TLB approaches as it offers a unified evolution equation for all the media in a physical system. The evolution equation [Eq. 2.30] comprises an additional collision operator included into the conventional simplified thermal lattice-Boltzmann (STLBM)

method which is dictated by the volume fraction of the solid medium and facilitates a smooth transition of boundary conditions at the solid-fluid interface. From the in-depth survey of literature presented in Chapter 1, one may conclude that several researchers have explored the IB-TLB method at length. However, investigations using the PSC methodology for heat transfer problems are very limited, even though it possesses appealing potential to simulate incompressible flows. Hence, in the present chapter, a critical assessment of the thermal-PSC model with respect to its order of accuracy, Galilean invariance, and efficacy of the solver for thermal problems are presented. The remainder of the chapter is organized as follows. Section 4.1 and 4.2 highlights the accuracy and Galilean invariance of the method. Furthermore, the method is carefully examined in a wide range of benchmark test cases in Section 4.3, which include different types of heat transfer phenomena along with stationary, imposed, and induced motion of the particle. Finally, the salient conclusions of all-encompassing analysis and directions for future efforts are summarized in Section 4.4.

4.1 Accuracy Study

This section is devoted towards examining the order of accuracy of the thermal-PSC algorithm for moving boundary problems. It should be mentioned here that an accuracy study reported by Chen and Müller [80] is presented for Eq. 2.31 to a conduction-dominated flow. However, the present study focuses on convection dominating cases and, in particular, showcases the algorithm's accuracy pertaining to moving straight and curved boundaries. Initially, the thermal Couette flow with wall injection is solved and its accuracy is compared with respect to the thermal lattice Boltzmann method (TLBM). Then, the cylindrical thermal-Couette flow is investigated to evaluate the algorithm's accuracy when subjected to complex boundaries which are not aligned with the underlying Cartesian mesh.

4.1.1 Thermal Couette flow with wall injection

The schematic representation of the thermal Couette flow with wall injection is illustrated in Fig. 4.1 along with the hydrodynamic and thermal boundary conditions. The periodic boundary condition at left and right computational boundaries is provided for both hydrodynamic and thermal governing equations. The Reynolds number based on the height of the channel (H) and injection velocity (V_0) is set as $Re = v_0 H / \nu_f = 10.0$. In order to conduct the spatial accuracy test, the number of lattice nodes on channel height are varied from 20 to 160, the relaxation time is set to $\tau_f = 1.0$, Prandtl number $Pr = 0.71$ and the physical parameters are set identical for all cases as : channel

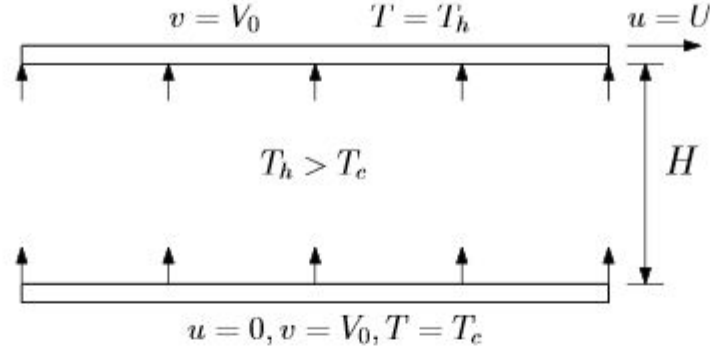


Figure 4.1: Schematic representation of thermal Couette flow with wall injection.

height ($H = 10^{-3}m$) and kinematic viscosity of fluid ($\nu = 10^{-6}m^2/s$). The simulations are run until the velocity and temperature errors are converged at 10^{-8} as per the Eq. (4.1).

$$\text{Convergence criteria} = \left| \frac{\text{err}(t)}{\text{err}(0)} \right| \quad (4.1)$$

where, $\text{err}(t)$ and $\text{err}(0)$ represent the root-mean-squared error at any instant (t) and the initial error value at $t = 0$, respectively. The analytical velocity and temperature profile of the flow field is expressed as:

$$U^{ana} = U \left[\frac{\exp(Re.y/H) - 1}{\exp(Re) - 1} \right] \quad (4.2)$$

$$T^{ana}(y) = T_c + \left[\frac{\exp(Re.Pr.y/H) - 1}{\exp(Re.Pr) - 1} \right] \Delta T \quad (4.3)$$

The primary objective of this study is to assess the accuracy of thermal-PSC models. To facilitate the same, extra layers of solid cells are added beyond top and bottom boundaries. The pure solid cells and solid-fluid interface cells are assigned volume of body (Φ_B) as 1.0 and 0.5, respectively. L_∞ and L_2 error norms are evaluated in the entire computational domain as:

$$L_\infty \text{ error} = \max |T^{ana} - T^{num}|, \forall \Phi_B < 1.0 \quad (4.4)$$

$$L_2 \text{ error} = \sqrt{\frac{1}{N} \sum_{\forall \Phi_B < 1.0} |T^{ana} - T^{num}|^2} \quad (4.5)$$

where, N denotes number of lattice nodes in that range and T^{ana} and T^{num} represent analytical and numerical solutions of temperature, respectively. The TLBM exhibits first and second order accurate spatial convergence in L_∞ and L_2 temperature errors respectively, as shown in Fig. 4.2a.

It should be mentioned here that the present TLBM solver exhibits quadratic

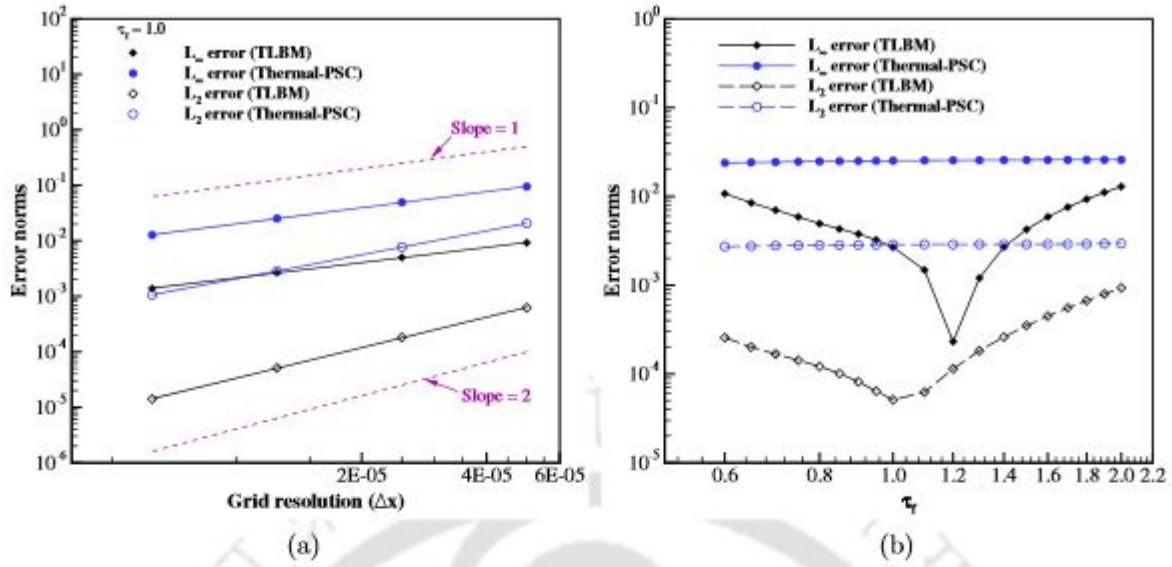


Figure 4.2: (a) Variation of temperature error norms with respect to (a) grid resolution (Δx) and (b) varying τ_f for thermal Couette flow with wall injection.

spatial convergence in maximum relative temperature error when evaluated over a single plane perpendicular to the flow direction, which is in well accordance with the study of Liu et al. [86]. Thermal-PSC solver converges with at least first-order rate with respect to the grid refinement. The asymptotic analysis of Eq. (2.31) as proposed by Chen and Müller [80] revealed it to be a second-order scheme; however, the analysis was solely carried out for a solid-fluid interface cell. In addition to it, they reported the scheme to be second-order accurate in temperature errors by undergoing numerical simulations in a conduction-dominated flow. A best-fit curve through the discrete data points of the relative error plot of the study reported by Chen and Müller [80] reveals approximately 1.5 order of convergence rate with respect to grid refinement. The present analysis reveals that the thermal-PSC algorithm converges approximately at a rate of 1.42 with grid refinement in L_2 error norms for a convection-dominated test case. A similar trend in the order of accuracy of these models is observed using $\tau_f = 0.6$, however, the plots pertaining to it are not shown for the brevity of the thesis. Further a τ_f sensitivity test is conducted in the range $[0.6, 2.0]$ while fixing the number of lattice nodes on channel height to 80, to re-assure the influence τ_f in the thermal-PSC model. Fig. 4.2b shows, the TLBM errors decrease till $\tau_f = 1.2$ and 1.0 for L_∞ and L_2 errors respectively, and further increase with respect to τ_f . The TLBM possesses at-least one decade smaller magnitude of error than the thermal-PSC algorithm. The thermal-PSC model is apparently insensitive to the choice of τ_f and exhibits identical order of magnitude of errors across the range of τ_f . However, the τ_f sensitivity of the model needs to be further explored in the context of moving boundary problems

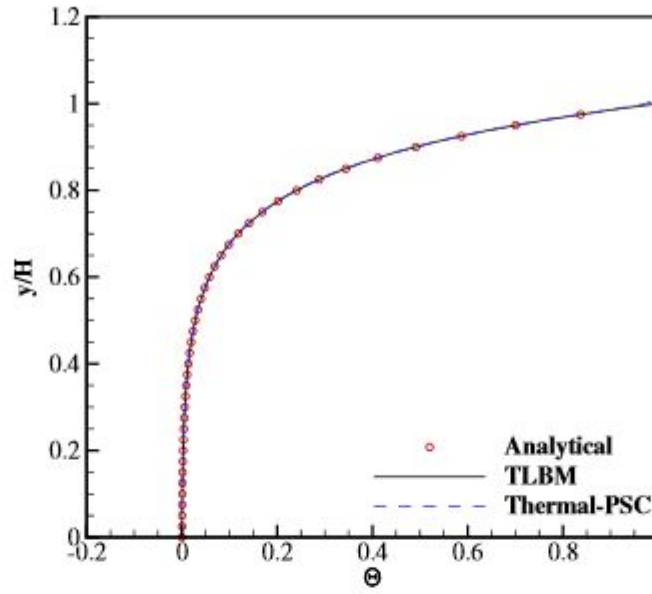


Figure 4.3: Temperature profile of thermal Couette flow with wall injection.

and other types of heat transfer processes. To ascertain the accuracy of the models in prediction of the temperature profile across channel width, non-dimensionalized temperature profiles ($\Theta = (T - T_c)/(T_h - T_c)$) are plotted against the analytical solution [Eq. (4.3)] in Fig. 4.3. Even though TLBM and thermal-PSC model exhibit good proximity of numerical profile with the analytical solution, a temperature jump is evident on the moving wall at $y/H = 1.0$ for the thermal-PSC model, which is inherent to immersed-boundary methods [65, 73].

4.1.2 Cylindrical thermal-Couette flow

The present subsection examines the accuracy of the thermal-PSC algorithm applied to two-dimensional cylindrical Couette flow between two circular cylinders for Dirichlet boundary conditions. The motivation behind choosing this test case is to analyze the PSC algorithm for immersed structures that are not aligned with the underlying regular Cartesian mesh and have curved surfaces, unlike the preceding test case. As depicted in Fig. 4.4, 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 Ω_P , and the outer cylinder remains static. The inner and outer cylinders are provided with constant hot and cold temperatures as $T_1 = 1$ and $T_2 = 0$, respectively. Note that the cylinders in the present study are placed in a computational domain of size $L \times L$, and the grey shaded part shown in Fig. 4.4 represents the solid part with temperature according to the adjacent cylinder temperature. The non-dimensional parameters for this problem are defined and set as : Reynolds number ($Re = (R_1 \Omega_P)(2R_1)/\nu_f = 10$)

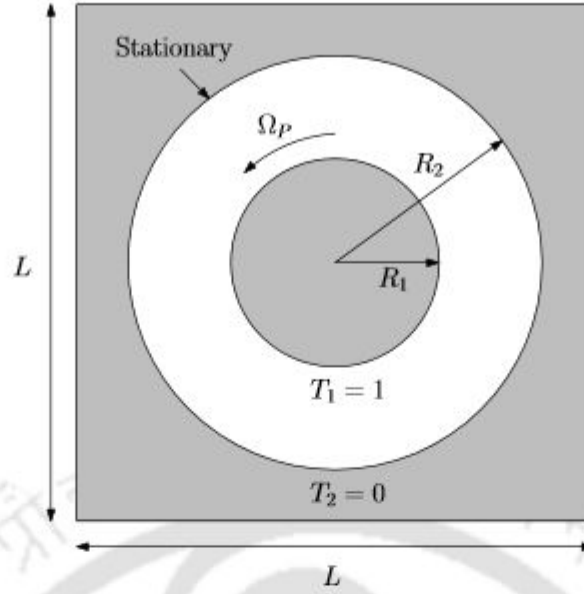


Figure 4.4: Computational domain for cylindrical thermal-Couette flow.

and Prandtl number ($Pr = \nu_f/\chi_f = 0.73$). The spatial order of accuracy test of the solver is performed by varying grid size as $\Delta x = L/40, L/80, L/160, L/320$ and constant relaxation time (τ_f) at 1.0. The L_∞ and L_2 errors for temperature are determined using expressions (4.4) and (4.5). The analytical solution for temperature is evaluated as

$$T^{ana} = T_2 - (T_2 - T_1) \frac{\ln(r/R_2)}{\ln(R_1/R_2)} \quad (4.6)$$

The convergence criterion [Eq. (4.1)] for these simulations is set to be 10^{-8} . Fig. 4.5a shows the spatial convergence of L_∞ and L_2 error norms of temperature. The thermal-PSC method shows first-order accurate grid convergence. This finding is in coherence with other IB-TLB models [66, 71, 73]. Temperature error norms of the model at different values of τ_f and fixed grid resolution ($\Delta x = L/80$) are depicted in Fig. 4.5b. Interestingly, for a complex boundary scenario, the thermal-PSC model exhibits an increase in error norms with an increase in τ_f . Nevertheless, the temperature profile produced by the thermal-PSC model in the flow field is in excellent agreement with respect to its analytical solution, as depicted in Fig. 4.6. An inevitable temperature jump at the solid-fluid interface, especially close to the moving surface, is also evident in the figure. The present and former sections dictate that the thermal-PSC model is approximately insensitive to the choice of τ_f for straight boundaries but responds to it in a curved boundary problem. It also exhibits first-order accurate spatial convergence irrespective of straight or curved boundaries. However, these inferences must not be construed at this stage to justify the model's suitability for thermal flows. Its efficacy needs to be investigated further in the context of predicting local heat transfer characteristics under different types of heat transfer processes illustrated in subsequent

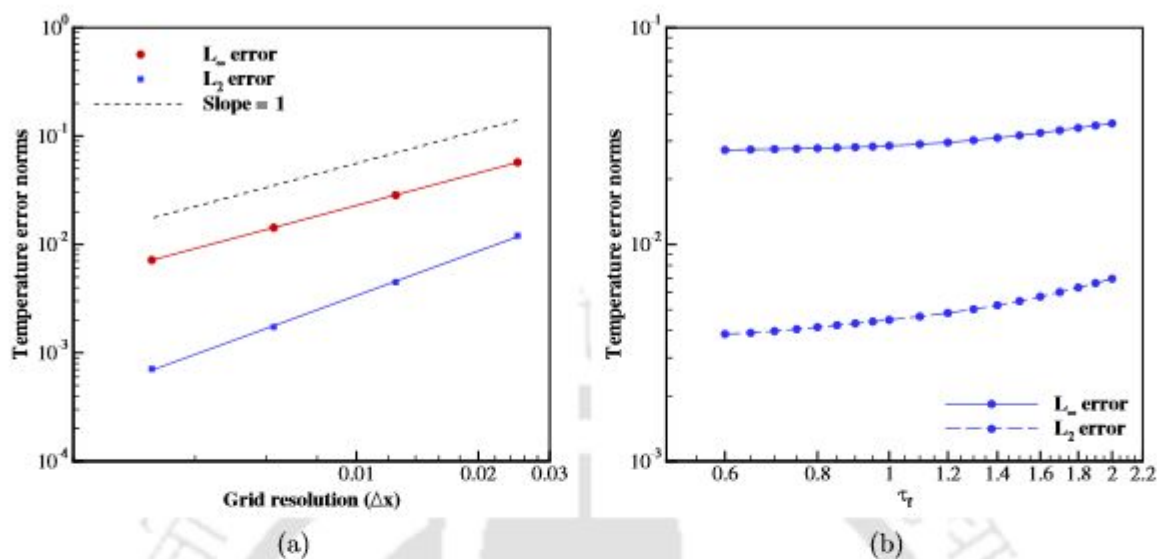


Figure 4.5: (a) Variation of temperature error norms with respect to grid resolution and (b) variation of error norms of temperature with respect to varying τ_f for cylindrical Couette flow.

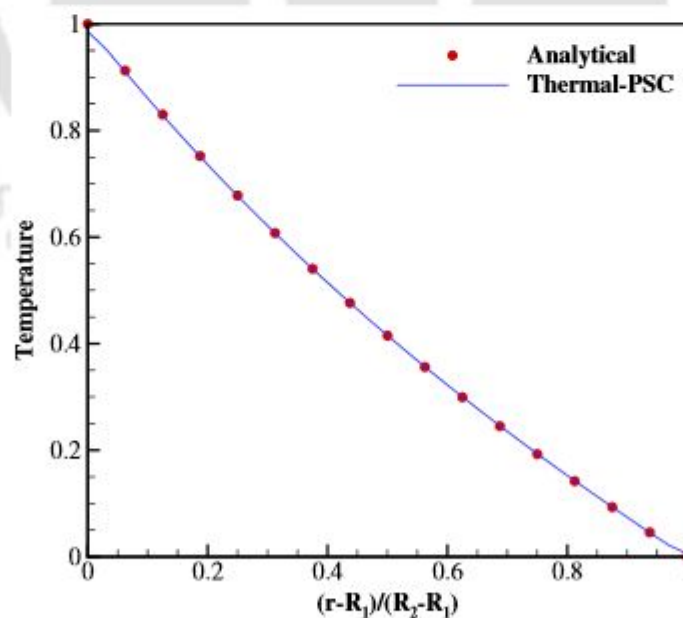


Figure 4.6: Comparison of temperature profile of cylindrical Couette flow between thermal-PSC and analytical solution.

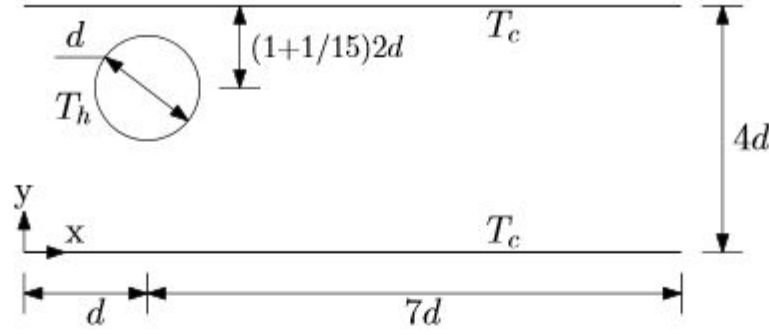


Figure 4.7: Schematic of a cylinder in a Couette flow.

sections.

4.2 Galilean invariance study

So far it is established that, thermal-PSC model is atleast first order accurate for moving boundary problems irrespective of the boundaries being straight or curve. In addition to the accuracy study, Galilean invariance is also a study of paramount importance particularly for moving boundary problems. It ensures that the computational method will produce identical flow field irrespective of the choice of reference frame being stationary or moving. A recent study by Haussmann et al. [51] shows the hydrodynamic PSC method is Galilean invariant. However, the thermal-PSC method has not been tested for the same to the best of the authors' knowledge. To facilitate this study, numerical simulation of transient Couette flow past a heated circular cylinder is conducted. The schematic and parameters of the test case is inspired by the work of Lallemand and Luo [34] and shown in Fig. 4.7. A heated circular cylinder of diameter $d = 0.05m$ is maintained at constant temperature T_h , while the top and bottom boundaries are provided lower temperature T_c . The simulations of stationary reference frame is facilitated by providing the initial flow field (U_0) and moving cylinder's velocity (U_c) in x -direction as $0.02m/s$. The top and bottom boundaries of the channel are moving opposite to each other with velocity (U_w) $0.1m/s$ in x -direction. The hydrodynamic and thermal boundary conditions at LB-level for top and bottom boundaries are implemented using methods proposed by Zou and He [11] and Liu et al. [86], respectively, while periodic boundary conditions are applied on the left and right boundaries. The moving reference frame simulations are conducted by adopting a constant reference velocity ($U_{ref} = -0.02m/s$) in the x -direction. Hence, the initial flow field becomes quiescent ($U_0 + U_{ref} = 0.0m/s$) and cylinder stays static ($U_c + U_{ref} = 0.0m/s$). The resultant velocity of the top and bottom boundaries becomes ($U_w + U_{ref} = 0.08m/s$) and ($U_w + U_{ref} = -0.12m/s$) respectively. The non-dimensional parameters for these simulations are set as $Re = d^2\kappa/\nu_f = 11.36$, $Pr = 0.7$ and $\tau_f = 0.714$. The shear

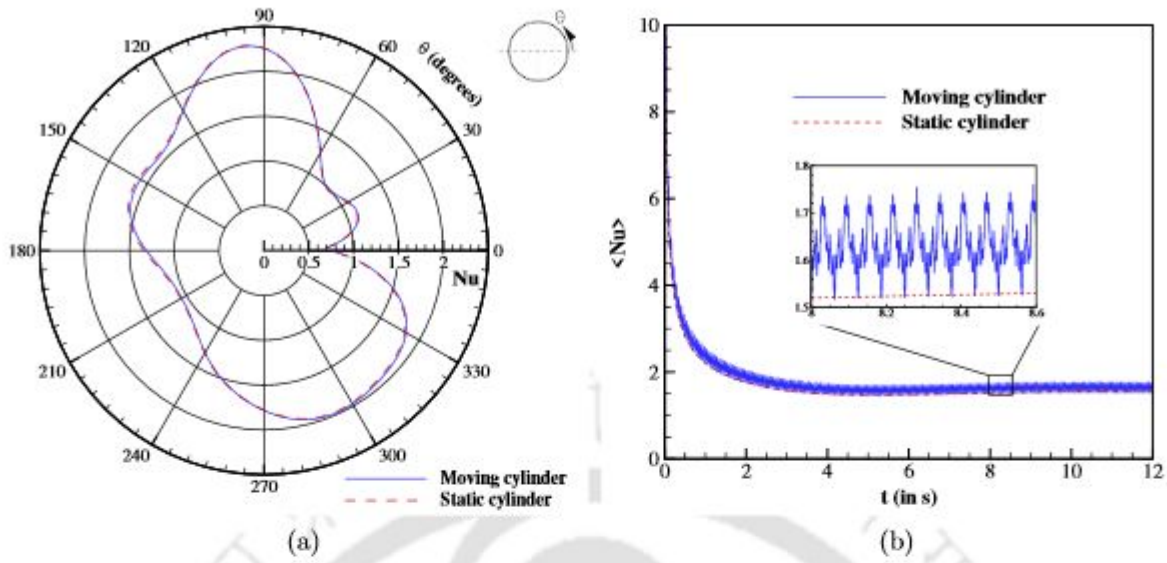


Figure 4.8: Variation of (a) local Nusselt number distribution as a function θ at time ($t = 10.0s$) and (b) average Nusselt number as a function of time.

rate of the flow is represented as $\kappa = 2U_w/4d$. Fig. 4.8a shows the local Nusselt number distribution over the cylinder's surface at time, $t = 10.0s$. The distribution of the Nusselt number is not symmetrical, which can be attributed to the asymmetrical placement of the cylinder between the plates. It can be observed that the moving and static cylinder cases reveal an excellent match amongst themselves, which in turn asserts the method to be Galilean invariant. The accuracy of the thermal-PSC model in predicting temperature field and Nusselt number for varied class of problems will be dealt with in detail in the subsequent section.

The time evolution of average Nusslet number ($\langle Nu \rangle$) (shown in Fig. 4.8b) also suggests that the values obtained in moving and static cylinder cases are almost identical for thermal-PSC model. To ratify the observation, the L_2 -normed difference (Δ_2) of local and average Nu between moving and static cylinder cases are evaluated. The Δ_2 expressions for local and average Nu , are respectively given as

$$\Delta_2(\text{local } Nu) = \sqrt{\frac{\sum_i ||Nu_m(\theta_i) - Nu_s(\theta_i)||^2}{\sum_i ||Nu_s(\theta_i)||^2}} \quad (4.7)$$

$$\Delta_2(\langle Nu \rangle) = \sqrt{\frac{\sum_t ||Nu_m(t) - Nu_s(t)||^2}{\sum_t ||Nu_s(t)||^2}} \quad (4.8)$$

where, the subscripts m and s , represent moving and static cylinder cases, respectively. The Δ_2 magnitude of local Nu at an instant $t = 10.0s$, and average Nu in the period $9.0s \leq t \leq 10.0s$ is 1.98×10^{-4} and 7.70×10^{-2} , respectively. Such low order of

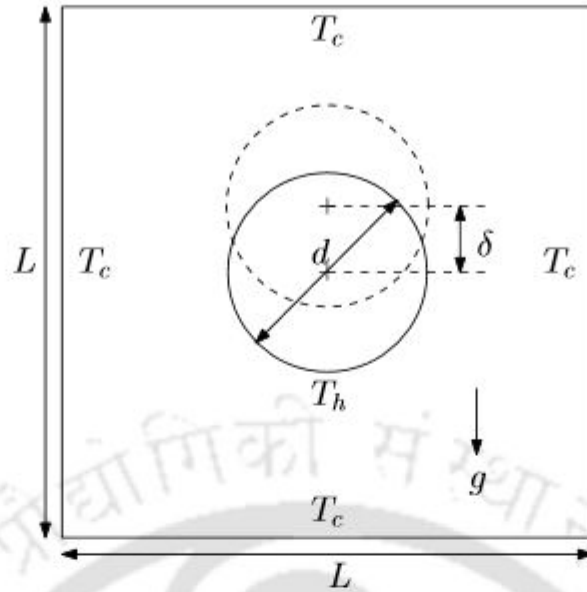


Figure 4.9: Schematic of an eccentrically placed heated circular cylinder inside a cold cavity

magnitude of Δ_2 suggests that the thermal-PSC model can be concluded as Galilean invariant.

4.3 Validation of benchmark problems using thermal-PSC

The accuracy and Galilean invariance studies presented so far have established that the thermal-PSC method is a promising framework for carrying out heat transfer simulations. However, a formal benchmarking of the method is imperative to establish its robustness and efficacy. The present section carries out a validation study for a wide spectrum of test cases encompassing natural, mixed, and forced convection phenomena that also involve stationary and moving structures. In addition to it, the performance of the solid collision operator is examined while evaluating the local flow field and heat transfer characteristics.

4.3.1 Natural convection of heated circular cylinder inside cold cavity

Numerical simulation of natural convection of an eccentrically placed heated circular cylinder inside a cold cavity is presented in this section. A stationary circular cylinder having diameter d is immersed into a square cavity of size L , such that $d = 0.4L$ as represented in Fig. 4.9. The cylinder is eccentrically placed at a distance δ , measured

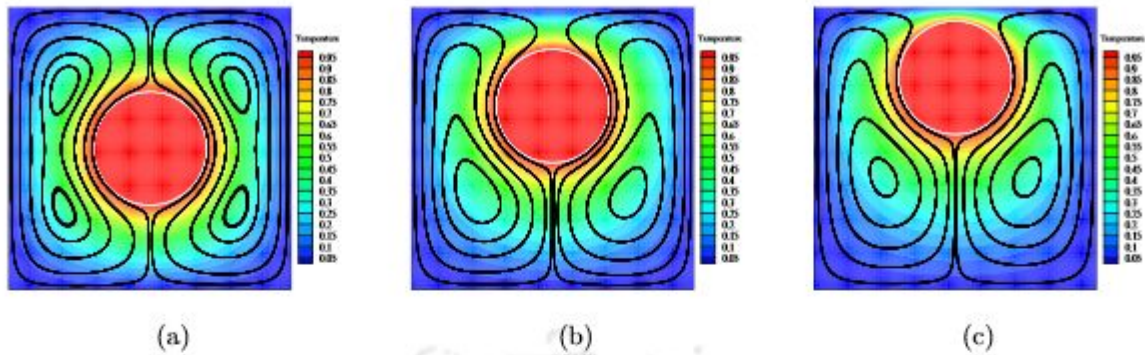


Figure 4.10: Streamline and temperature distribution contours of natural convection of circular cylinder inside a cavity at $Ra = 10^3$ and cylinder offset (a) $\delta = 0.0$, (b) $\delta = 0.15L$ and (c) $\delta = 0.25L$.

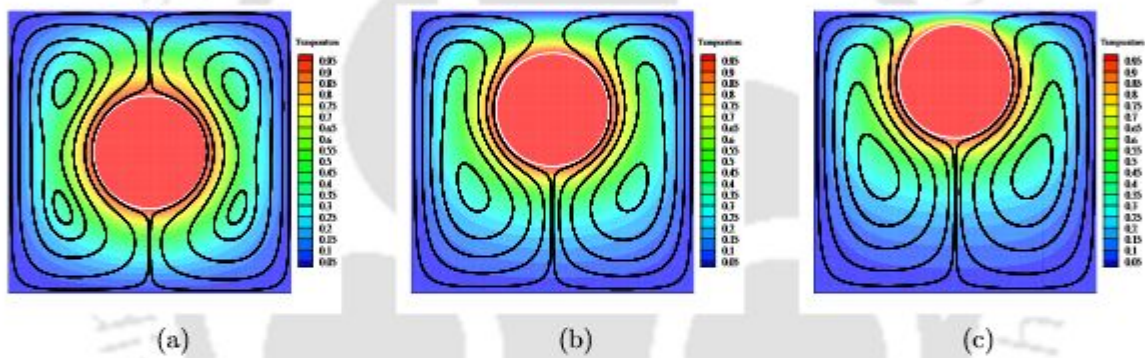


Figure 4.11: Streamline and temperature distribution contours of natural convection of circular cylinder inside a cavity at $Ra = 10^4$ and cylinder offset (a) $\delta = 0.0$, (b) $\delta = 0.15L$ and (c) $\delta = 0.25L$.

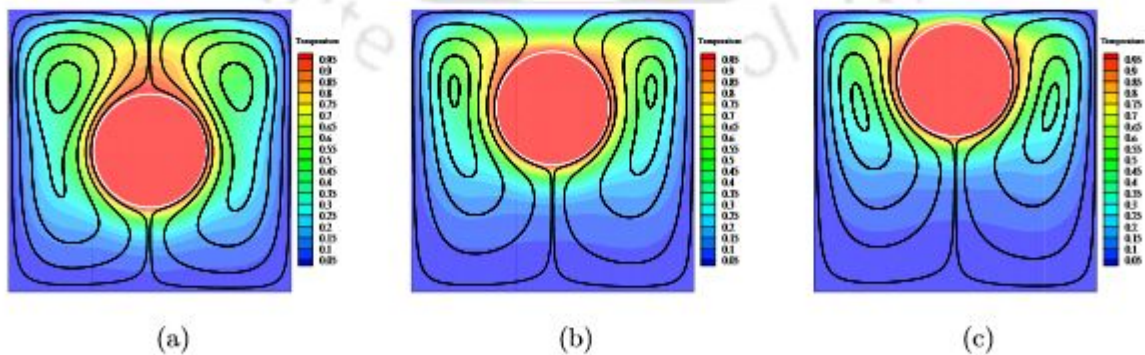


Figure 4.12: Streamline and temperature distribution contours of natural convection of circular cylinder inside a cavity at $Ra = 10^4$ and cylinder offset (a) $\delta = 0.0$, (b) $\delta = 0.15L$ and (c) $\delta = 0.25L$.

in positive y -direction from the domain center. The cylinder is provided Dirichlet type higher temperature T_h , whereas the initial temperature and cavity boundaries are set to lower temperature T_c . The temperature boundary conditions at cavity walls are incorporated as discussed in Liu et al. [86] while no-slip boundary conditions at the enclosure walls are set following the Zou/He boundary conditions [11]. The temperature difference between the circular cylinder and enclosure walls triggers natural convection in the enclosure, and the fluid experiences buoyant force. This body force density is evaluated using Boussinesq approximation [Eq. (2.12)], where T_0 is taken as the average of T_h and T_c . Non-dimensional parameters are set as $Pr = 0.7$, Rayleigh numbers $Ra = 10^3, 10^4, 10^5$ while varying the cylinder location according to $\delta = 0.0, 0.15L, 0.25L$. The computational domain is constituted of uniform rectangular lattices of size 151×151 , 251×251 and 551×551 for $Ra = 10^3, 10^4$ and 10^5 respectively. The above choices of grid size are based on grid-independent solutions of respective Rayleigh numbers. The relaxation time τ_f is set to 0.75 for all the cases of the Rayleigh number. The parameters are carefully selected so as to ensure the flow within the incompressible limit of Mach number (Ma) < 0.3 . The viscosity and thermal diffusivity of the fluid is related to the non-dimensional parameters in natural convection problems as

$$\nu = \sqrt{\frac{Pr}{Ra}} U_c L \quad (4.9a)$$

$$\alpha = \frac{U_c L}{\sqrt{Ra Pr}} \quad (4.9b)$$

$$U_c = \sqrt{\beta g \Delta T L} \quad (4.9c)$$

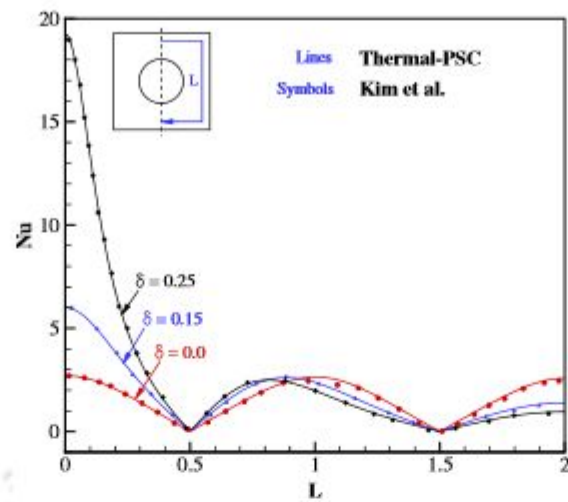
Here, U_c, L and ΔT represent characteristic velocity, length, and temperature difference ($T_h - T_c$), respectively. Steady state solution for the present simulation is obtained by setting convergence criteria to 10^{-10} .

Fluid adjacent to the hot circular cylinder gradually gets warmer and moves upward to touch the cold cavity at the top. It subsequently cools down and becomes denser to descend along the cold cavity wall while simultaneously forming two symmetric free circulations in the cavity. Fig. 4.10, 4.11 and 4.12 shows streamline and temperature contours at different cylinder locations for $Ra = 10^3, 10^4$ and 10^5 respectively. At $\delta = 0.0, Ra = 10^3$, the flow is conduction dominant, and the circulation displays two symmetrically rotating vortices. Circulation inside the cavity at $\delta = 0.0, Ra = 10^4$ exhibits a similar pattern as compared to that at $Ra = 10^3$, while a closer observation reveals that thermal boundary layer at bottom part of the cylinder is thinner than that at the top of the cylinder. Moreover, the vortex at the lower part of the cylinder is weaker and smaller than its counterpart at the top. This is because of the fact that,

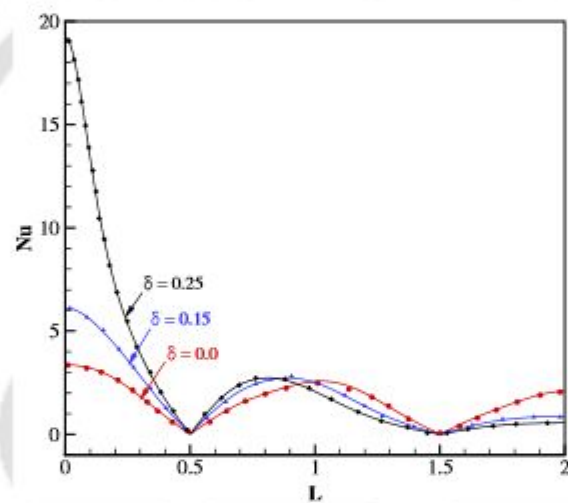
at a higher Rayleigh number, convection heat transfer takes over the conduction mode of heat transfer. As the Rayleigh number increases to $Ra = 10^5$, $\delta = 0.0$, convection heat transfer becomes dominant in the cavity resulting in a thinner thermal boundary layer along the inner cylinder surface. It is observed that a plume is formed at the top of the cylinder which gives rise to a stronger gradient there in contrast to a weaker thermal gradient at the cylinder bottom. In addition, the merger of two inner vortices leads to a dominant flow and recirculating eddies at the top of the cylinder in contrast to the lower Rayleigh number cases. Weak flow at the bottom region of the cavity reveals stratification of the flow in this region.

When the cylinder advances in the positive y -direction at $Ra = 10^3$, the space between the cylinder surface and cavity wall decreases at the top, which results in a gradual decrease in size of the upper vortex and finally merges into a single vortex at the lower part of the cavity. Moreover, as the Rayleigh number increases, the vortex's size increases and its core moves towards the center of the cavity. The isotherm contours reveal that, as δ increases, they appear denser at the top of the cylinder than the bottom part giving rise to a high thermal gradient at the top. A similar trend like $Ra = 10^3$ is also observed for $Ra = 10^4$ while moving the cylinder in the upward direction. The effect of convection heat transfer is more in this case as compared to the $Ra = 10^3$. A cold stagnation region with poorer heat transfer is observed at the bottom of the cylinder compared to strong convective heat transfer at the cylinder top. While increasing δ in positive y -direction at $Ra = 10^5$ similar scenario of single recirculation region is observed as in $\delta = 0.0$. As the space between the cylinder and top wall of the cavity narrows, the locally conductive mode of heat transfer dominates over the convective heat transfer due to the restricted vertical motion of the flow. These isotherm and streamline contours are in well agreement with the observations made by Kim et al. [115].

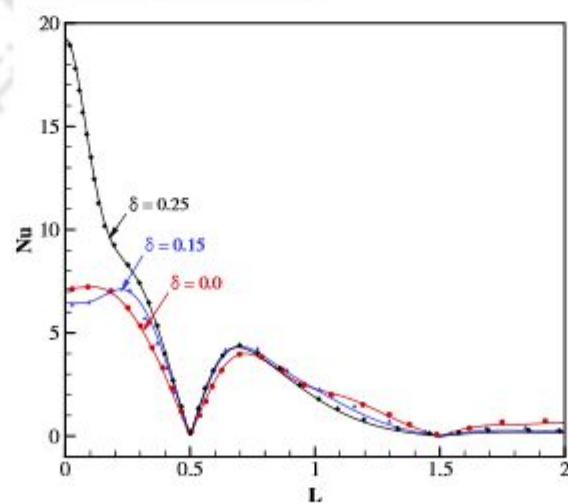
Fig. 4.13 shows the local Nusselt number over the cold cavity's surface (only the right half of the domain is shown because of the symmetry) for different cylinder locations and Rayleigh numbers. Fig. 4.14 shows local Nusselt number over the hot cylinder's surface for $Ra = 10^3, 10^4$ and 10^5 . The angle θ starts at the top of the cylinder at the vertical centerline and increases in the clockwise direction. At $Ra = 10^3, \delta = 0.0$, Nusselt number variation is large at cavity surface as compared to the cylinder surface. Whereas, in both the cases symmetric variation of Nusselt number due to conduction dominant flow field is observed. Fig. 4.13a also reveals that Nu at mid-length of the top surface of the cavity is maximum for the location being the stagnation point. It decreases towards the right and attains a minimum at the top right corner of the cavity. As one traverses down along the surface, Nu increases till it attains maximum value at the mid-length of the right surface and



(a)

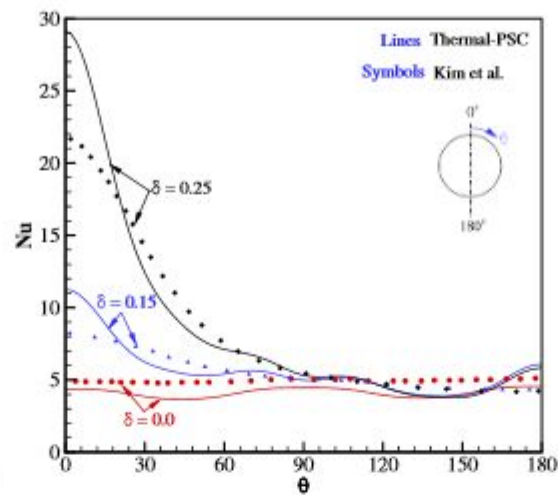


(b)

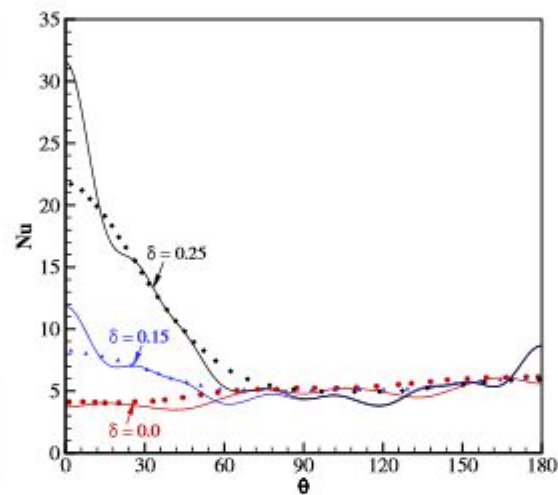


(c)

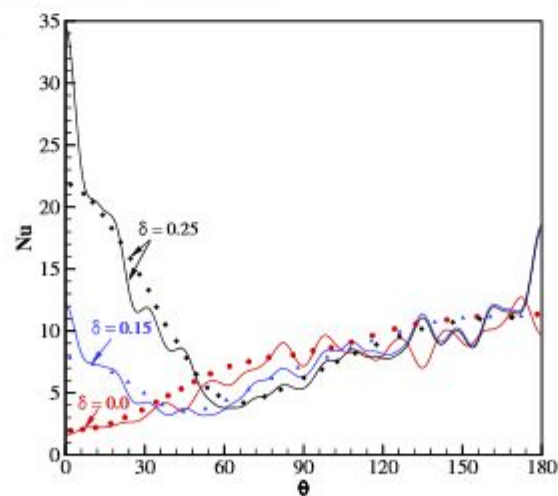
Figure 4.13: Comparison of local Nusselt number along the cavity's surface with Kim et al. [115] at (a) $Ra = 10^3$, (b) $Ra = 10^4$ and (c) $Ra = 10^5$.



(a)



(b)



(c)

Figure 4.14: Comparison of local Nusselt number along the cylinder's surface with Kim et al. [115] at (a) $Ra = 10^3$, (b) $Ra = 10^4$ and (c) $Ra = 10^5$.

subsequently decreases again till the bottom right corner of the cavity. As the cylinder advances in the positive y - direction, symmetry of the domain along $y = 0$ is lost and so as the Nu variation along the cavity and cylinder's surface. With increase in δ , the space between cylinder and cavity's top surface becomes narrower that results into higher thermal gradient for higher δ at $0^\circ \leq \theta \leq 90^\circ$ and again subsequently decrease at $90^\circ \leq \theta \leq 180^\circ$ as compared to $\delta = 0.0$ (Fig. 4.14a). Similarly, the local Nusselt number variation for $0 \leq L \leq 1$ increases with increase in δ and decreases for $1 \leq L \leq 2$ with increase in δ as compared to the $\delta = 0.0$.

Fig. 4.13b and 4.14b reveal, Nusselt number increases with increase in Rayleigh number. The Nu variation at both the surfaces is not symmetric anymore at $\delta = 0.0$ as compared to $\delta = 0.0, Ra = 10^3$, which can be attributed to the increasing effect of convection heat transfer. With the increase in δ , variation of Nu along both the surfaces exhibit a similar pattern as observed in $Ra = 10^3$. Fig. 4.14c shows that, with an increase in δ for $Ra = 10^5$, the maximum value of Nu is observed above the cylinder at the constricted passage, which can be attributed to the strong thermal gradient at this location. Nu decreases gradually to a minimum value with an increase in θ , which further increases in the presence of the rising plume. It can also be observed that the location of minimum Nu also increases from top to bottom with an increase in δ due to the movement of the thermal plume in an increasing θ direction. As observed from Fig. 4.13c, the maximum value of Nu for $\delta = 0.15$ is less than any of the other cases considered here because of the prevailing upwelling and downwelling plumes and secondary eddies at the upper surface of the inner cylinder. Prediction of local Nu along the cavity's surface using the thermal-PSC method is in excellent agreement with that reported by Kim et al. [115]. However, thermal-PSC over-predicts the local Nu at location of high thermal gradients in comparison to Kim et al. [115], across all the variations of Ra and offset distance (δ) considered in the present work. This can also be attributed to the high oscillations of temperature gradient signals at that location and subsequent smoothening of the data.

4.3.2 Natural convection in a concentric cylinder

Buoyancy-driven flow with differentially heated surfaces in a concentric annulus is one of the basic phenomena in many engineering applications like energy management systems, heat exchangers, heating and cooling systems, etc. The present subsection demonstrates this system to reveal the capability of the solver to simulate curved boundary problems that are not aligned relative to the lattice mesh. As shown in Fig. 4.15, two concentric cylinders having radii R_i (inner cylinder radius) and R_o (outer cylinder radius) are immersed such that, $L = R_o - R_i$. The inner and outer

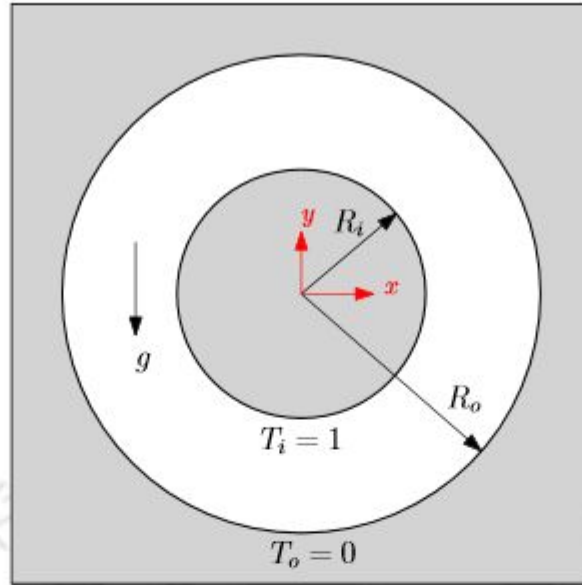


Figure 4.15: Schematic of computational domain for natural convection in an annulus subjected to Dirichlet boundary conditions.

cylinders are subjected to hot and cold Dirichlet-type temperature conditions as $T_i = 1$ and $T_o = 0$ respectively. The working fluid is confined between these cylinders and experiences a buoyancy effect due to natural convection, and the buoyant force is determined using Boussinesq approximation [Eq. (2.12)], where T_0 is taken as the average of T_h and T_c . Note that the shaded part in Fig. 4.15 is considered solid in the present solver, and the temperature in this region is set accordingly in consistent with the adjacent cylinder temperature. Governing non-dimensional parameters to this problem are set as: Prandtl number ($Pr = \nu_f/\chi_f = 0.7$), Rayleigh number ($Ra = (\mathbf{g}\beta\Delta TL^3)/(\nu_f\chi_f) = 5 \times 10^4$), and $L/D_i = 0.8$. Here, $D_i = 2R_i$ is the diameter of the inner cylinder. The computational domain is constituted of grid size 451×451 , 160 number of lattice nodes across the diameter of the inner cylinder, and the relaxation time is provided as $\tau_f = 0.6$. The problem is devised in such a way that the present simulation results can be compared with the experimental results of Kuehn and Goldstein [116]. Steady-state solution for the present simulation is obtained by setting convergence criteria to 10^{-10} .

Fig. 4.16 shows streamline and isotherm contours of the problem are in good agreement with the observation made by Kuehn and Goldstein [116]. It is also evident from the figure that, as the temperature of fluid near the hot inner cylinder boundary is more, the fluid rises up along the inner boundary and creates a plume at the center, while fluid adjacent to the outer boundary is relatively cold and thus moves downward along the outer cylinder. At such a high Rayleigh number, the natural convection of the fluid dominates, which results in a narrower plume of hot fluid at the top of the

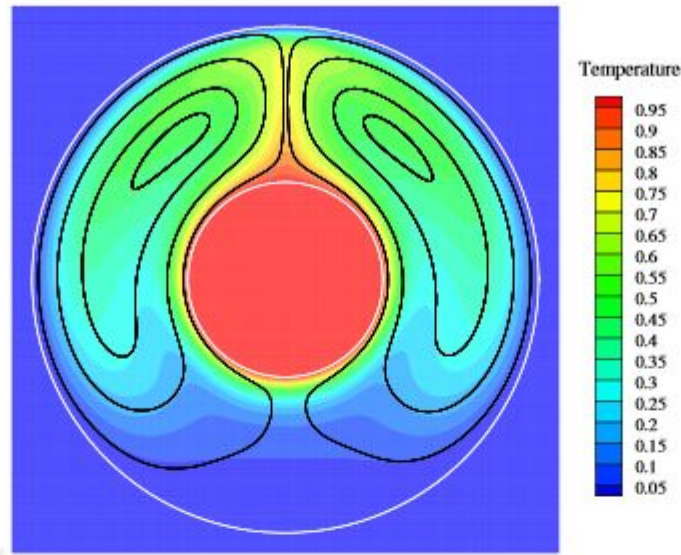


Figure 4.16: Streamline and temperature distribution contours of natural convection in an annulus at $Ra = 5 \times 10^4$

annulus.

Fig. 4.17 shows the dimensionless temperature distribution $[\Theta = (T - T_o)/(T_i - T_o)]$ as a function of non-dimensional radial distance $(r - R_i)/(R_o - R_i)$ in the annulus gap at different angles. The angles are measured from the positive y -direction and increase in the clockwise direction such that 0° and 180° are at the top and bottom of the cylinder, respectively. Fluid at the bottom of the inner cylinder exhibit the smallest thermal boundary layer thickness resulting in the largest temperature gradient and heat flux. As one moves from the bottom to the top of the cylinder, thermal boundary layer thickness increases gradually and creates a high-temperature gradient plume at the top of the cylinder. As the heat convection dominates in such a high Rayleigh number, it forms an inversion region such that fluid temperature near the outer cylinder is more than that near the inner cylinder. Fig. 4.17 and 4.18 clearly reveals the temperature and flow inversion between angles 30° to 90° .

The thermal-PSC model exhibits good agreement in angular velocity profile (Fig. 4.18) and temperature distribution with respect to the radial distance at various angles (θ) as compared to the experimental and numerical data obtained by Kuehn and Goldstein [116]. Fig. 4.19 shows the variation of local equivalent conductivity (k_{eq}) of both the cylinder boundaries. Local equivalent conductivity (k_{eq}) is defined as the ratio of local heat flux to the heat flux due to pure conduction in the absence of fluid motion. It can be depicted from the figure that k_{eq} for the inner cylinder is maximum at the bottom due to the maximum temperature gradient, and it gradually decreases from the bottom to the top of the cylinder owing to the minimum temperature gradient

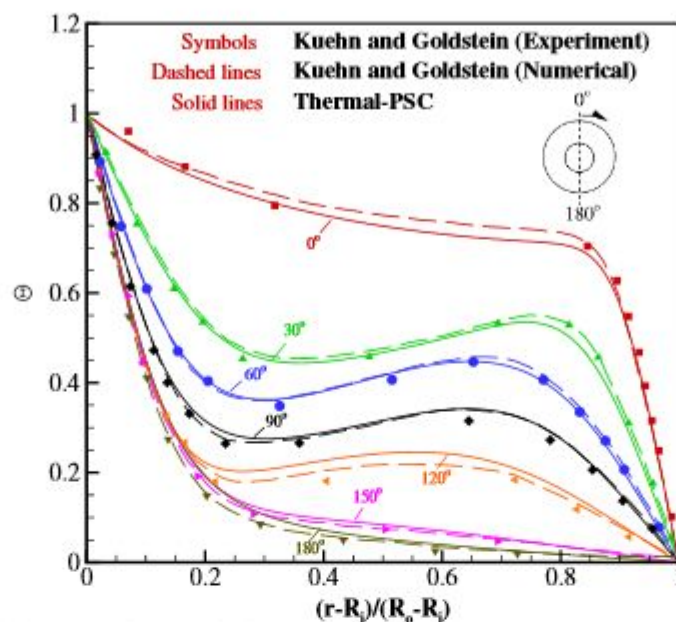


Figure 4.17: Comparison of dimensionless temperature distribution at different angles with Kuehn and Goldstein [116]. The numerical results are for $Ra = 5 \times 10^4$, $Pr = 0.7$ & $L/D_i = 0.8$ and the experimental results are for $Ra = 4.7 \times 10^4$, $Pr = 0.7$ & $L/D_i = 0.8$

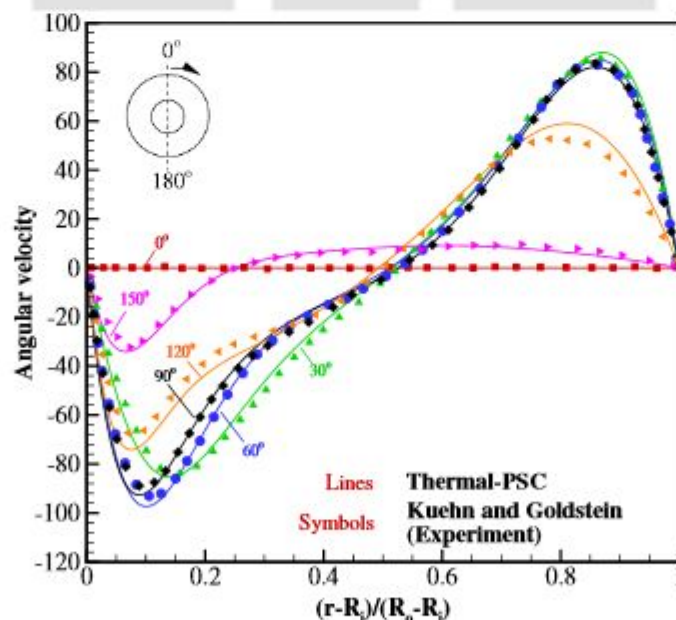


Figure 4.18: Comparison of angular velocity distribution at different angles for $Ra = 5 \times 10^4$, $Pr = 0.7$ and $L/D_i = 0.8$ with Kuehn and Goldstein [116].

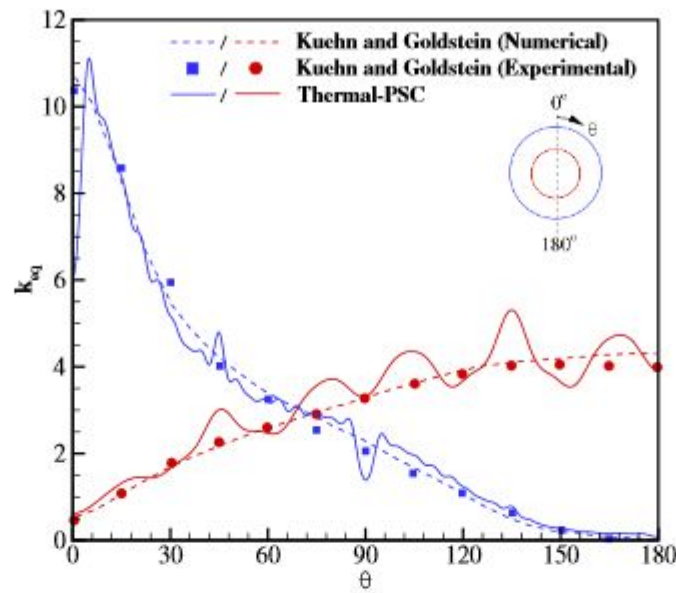


Figure 4.19: Comparison of local equivalent thermal conductivity with the numerical and experimental results of Kuehn and Goldstein [116]. The numerical results are for $Ra = 5 \times 10^4$, $Pr = 0.7$ & $L/D_i = 0.8$ and the experimental results are for $Ra = 4.7 \times 10^4$, $Pr = 0.7$ & $L/D_i = 0.8$

due to the impinging plume. In contrast to the inner cylinder surface, the outer cylinder surface experiences a maximum temperature gradient at the top resulting in higher k_{eq} and gradually decreases from top to bottom. The thermal-PSC model predicts a qualitatively correct trend of k_{eq} while maintaining the average value close to that reported by Kuehn and Goldstein [116]. In a nutshell, the preceding and the present test case on natural convection using thermal-PSC reveals that it is capable of predicting local temperature gradient over straight boundaries accurately but over-predicts at high thermal gradient location near curved surfaces.

4.3.3 Forced convection through an iso-thermally heated circular cylinder

Having investigated the natural convection phenomena using the thermal-PSC method, the present investigation steps towards appraising the efficacy of the PSC method for simulations of forced convection heat transfer processes involving complex boundaries. A forced convection heat transfer phenomenon over a heated stationary circular cylinder is investigated in this section. A circular cylinder having diameter d , is immersed at location $(18d, 20d)$ in a computational domain of size $40d \times 40d$ as represented in Fig. 4.20. A uniform velocity (U) flow field and lower temperature field ($T_c = 0$) are prescribed at the domain inlet. Higher temperature ($T_h = 1.0$) is imposed on the cylin-

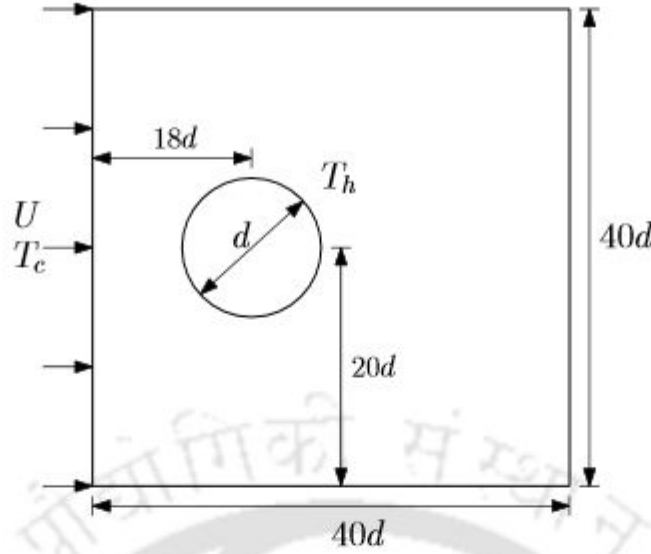


Figure 4.20: Schematic of computational domain for forced convection through an iso-thermally heated stationary circular cylinder.

der's surface. Constant pressure at outlet and slip boundary condition ($\partial u / \partial y = 0$ and $v = 0$) with adiabatic condition ($\partial T / \partial y = 0$) is applied at the top and bottom boundaries of the domain. The governing non-dimensional parameters for the test case are selected as Reynolds number ($Re = Ud/\nu_f = 20$) and Prandtl number ($Pr = \nu_f/\chi_f = 0.73$) so as to facilitate the comparison of present results with other numerical methods like arbitrary-Lagrangian-Eulerian (ALE) approach utilized by Gan et al. [117] and IB-TLB method used by Suzuki et al. [73]. 40 number of lattice nodes are put across the cylinder's diameter, and the relaxation time is chosen as $\tau_f = 0.7205$. It results in a free stream velocity $U = 0.03675$ in lattice units, which is well within the incompressible flow limit. The efficacy of the hydrodynamic-PSC solver for flow past a stationary circular cylinder is well reported in the previous work done by Owen et al. [48] and the preceding chapter of this thesis. Hence, the current investigation confines to examine the heat transfer characteristics only.

Fig. 4.21 shows the distribution of local Nusselt number over the heated cylinder's surface. The maximum value of the Nu is experienced at the front stagnation point of the cylinder, whereas the minimum is located at the rear. It can be attributed to a stronger temperature gradient at the front stagnation point, which is reflected in an isotherm contour as shown in Fig. 4.22. The thermal-PSC model exhibits excellent agreement in predicting local Nu distribution on the cylinder's surface with that of Gan et al. [117] and Suzuki et al. [73].

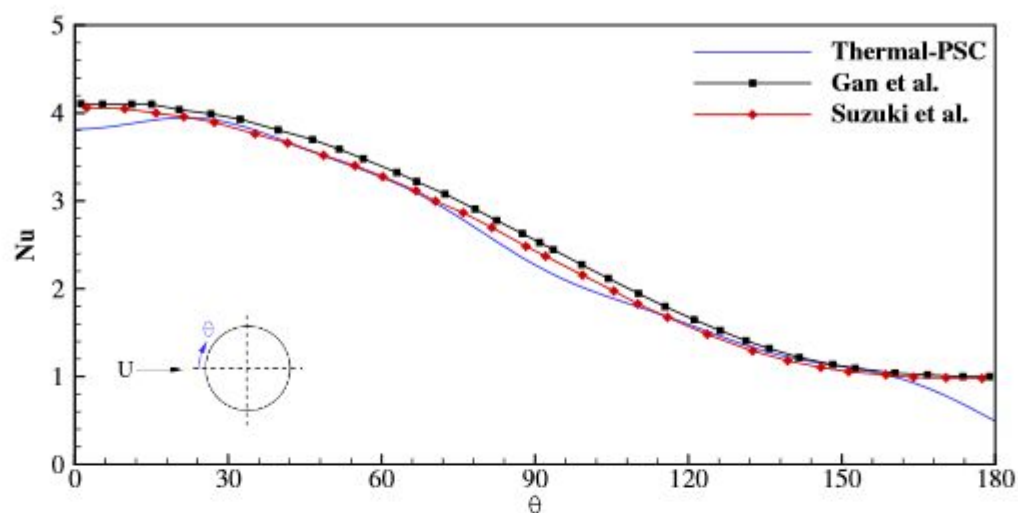


Figure 4.21: Distribution of local Nusselt number on the cylinder's surface for a forced convection over a heated circular cylinder at $Re = 20$ and its comparison with Gan et al. [117] and Suzuki et al. [73].

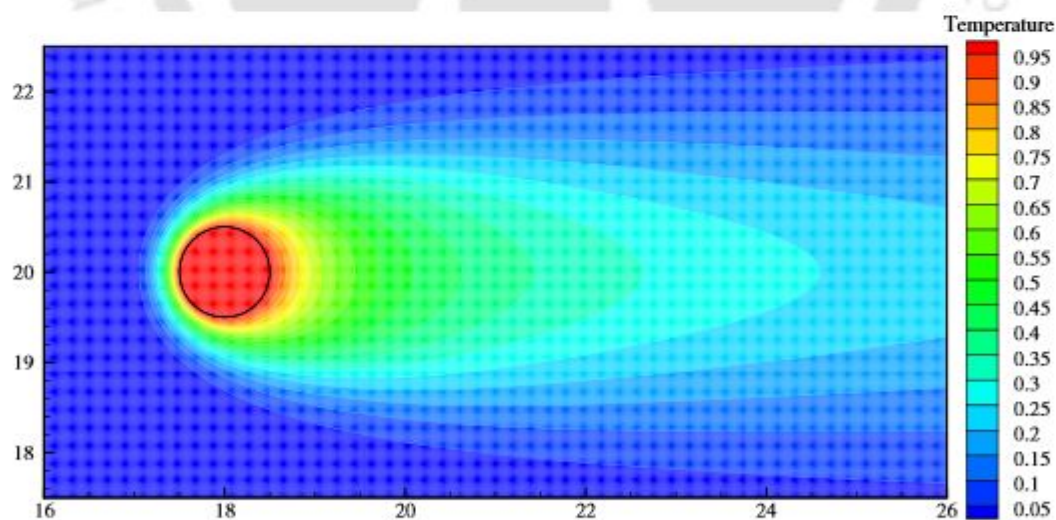


Figure 4.22: Isotherm contour for a forced convection over a heated circular cylinder at $Re = 20$.

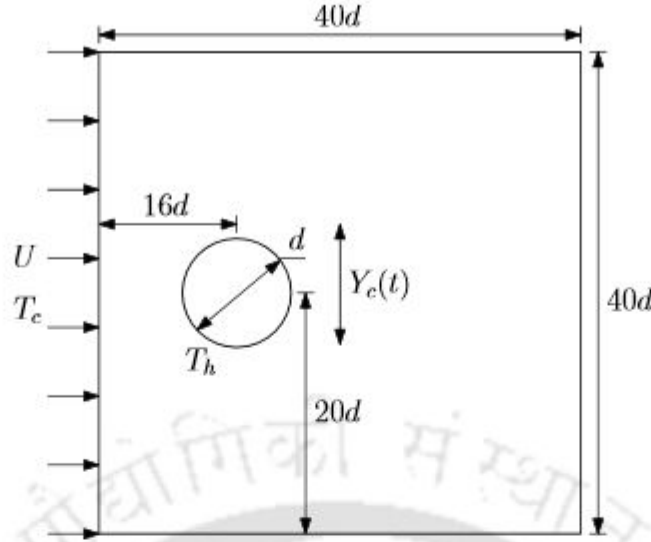


Figure 4.23: Schematic of computational domain for forced convection through a transversely oscillating heated circular cylinder.

4.3.4 Forced convection through transversely oscillating heated circular cylinder

The present section demonstrates the investigation of the thermal-PSC model when it is subjected to an imposed motion scenario and simultaneously undergoing forced convection heat transfer phenomena. A circular cylinder having diameter d , is embedded at location $(16d, 20d)$ in a computational domain of size $40d \times 40d$ as depicted in a schematic Fig. 4.23. The inlet and initial flow field of the computational domain are prescribed with a uniform velocity (U) and lower temperature ($T_c = 0.0$). The cylinder is subjected to a transverse oscillatory motion as $Y_c = A \sin(2\pi ft)$ and higher temperature ($T_h = 1.0$). The top and bottom boundaries of the computational domain are provided with zero velocity gradient conditions ($\partial u / \partial y = 0.0$ & $\partial v / \partial y = 0.0$) with adiabatic condition ($\partial T / \partial y = 0.0$). A constant pressure condition with an adiabatic heat transfer condition is applied at the domain's outlet. The governing non-dimensional parameters for the problem are chosen as: Reynolds number ($Re = Ud/\nu_f = 200$) and Prandtl number ($Pr = 0.7$). The amplitude (A) and frequency of cylinder's oscillation ($f = f_e/f_o$) are set to $0.15d$ and 0.2 , respectively. Here, f_e and f_o stand for the excitation frequency and natural vortex shedding frequency of the cylinder, respectively. It should be mentioned here that, in order to obtain the f_o , the Strouhal number ($St = f_o d/U$) for the flow past a stationary circular cylinder at $Re = 200$ is taken as 0.197 , which has been obtained a priori using the hydrodynamic solver in the preceding chapter. The LB level input parameters to the problem consist of 60 lattice nodes across the diameter of the circular cylinder, and relaxation time, τ_f is set to 0.59 . It also corresponds to the free stream velocity value as $U = 0.1$ lattice units,

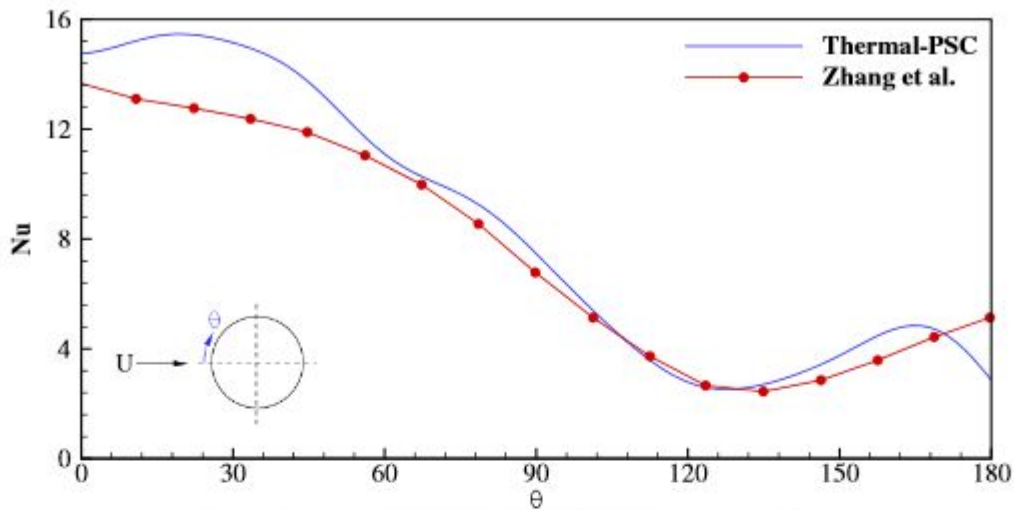


Figure 4.24: Distribution of local Nusselt number on the cylinder's surface for a forced convection over a transversely oscillating cylinder at $Re = 200$, $f = 0.2$ and $A = 0.15d$ and its comparison with Zhang et al. [61].

which confines the flow within the incompressible limit. The prediction of local Nusselt number over the cylinder's surface at $t = T/2$ (T =time period of oscillation), using the thermal-PSC model is in good agreement with the data obtained by Zhang et al. [61] and shown in Fig. 4.24. The maximum heat transfer is experienced at the front stagnation of the cylinder. The minimum heat transfer occurs at an approximate angle of 135° which is close to the flow separation point from where the vortex starts shedding. In a nutshell, the present and preceding forced convection problems that involve stationary and moving boundary scenarios suggest that the present thermal-PSC model can efficiently predict local heat transfer characteristics with finite accuracy, which is also in accordance with the studies reported by Chen and Müller [80].

4.3.5 Mixed convection in a lid-driven cavity with circular cylinder

This section investigates the efficacy of the thermal-PSC solver for the mixed convection problem. A circular cylinder having radius r is immersed into a lid-driven square cavity of side (H) such that $r = 0.2H$. The bottom wall of the cavity is prescribed at a higher temperature (T_h) as compared to the lower temperature (T_c) prescribed on the cylinder's surface and the top surface of the cavity. The top lid is moving with a constant speed (U) which corresponds to the Reynolds number of the flow inside the cavity as $Re = (UH/\nu_f) = 100$. The velocity and temperature boundary conditions used in this problem are represented in the schematic shown in Fig. 4.25. Non-dimensional parameters for the problem are chosen as: Prandtl number ($Pr = 0.7$), and Richard-

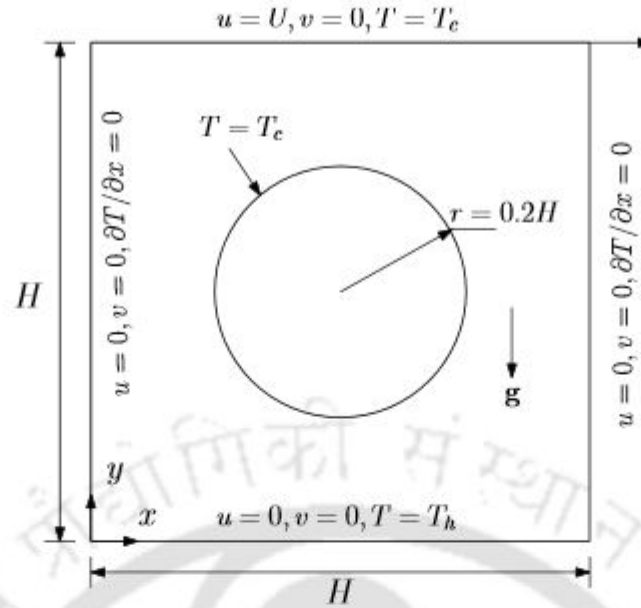


Figure 4.25: Schematic of mixed convection in lid-driven cavity with circular cylinder

son number ($Ri = Gr/Re^2 = 0.01, 1$ and 10). Here, Gr stands for the Grashof number and can be expressed as $Gr = Ra/Pr$. Fig. 4.26 shows the streamline and temperature distribution of the flow inside the cavity at various Richardson number (Ri). Higher Ri suggests a natural convection-dominated flow, which is evident from the expanded isotherms at the upper part of the cavity. Whereas low Ri signifies a forced convection-dominated flow wherein a recirculation vortex appears at the top of the circular cylinder. Higher Ri also instigates larger temperature gradient and eventually a larger heat transfer rate near the isothermal surfaces like the bottom and top wall of the cavity. Fig. 4.27 confirms this fact in terms of variation of local Nu over the heated surface. Moreover, the thermal-PSC solver shows good agreement with literature [118] across all the cases of Ri considered in this work. Determination of local Nu over the cylinder is a crucial objective of the present thesis. Due to the lack of open litera-

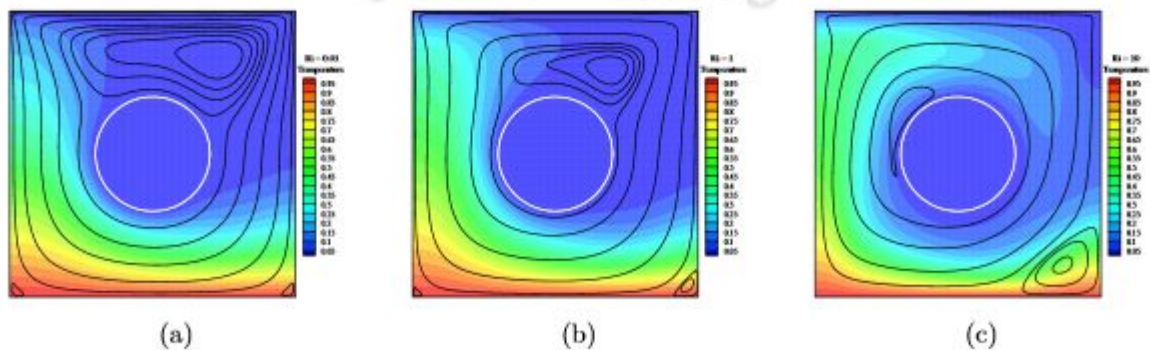


Figure 4.26: Streamline and temperature distribution contours of mixed convection in a lid-driven cavity with circular cylinder at (a) $Ri = 0.01$, (b) $Ri = 1$ and (c) $Ri = 10$.

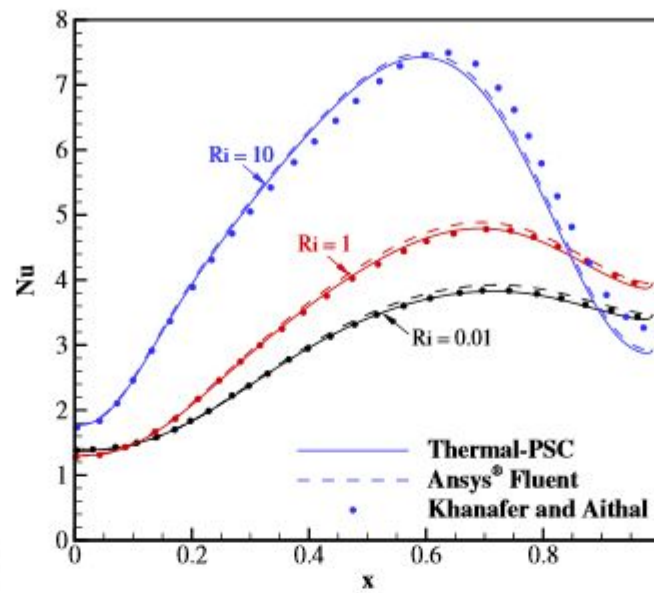


Figure 4.27: Comparison of local Nusselt number over heated wall with Ansys® Fluent and Khanafer and Aithal [118] at various Richardson number.

ture that provides such variation over the cylinder's surface, the same test cases are conducted in a commercial finite-volume framework Ansys® Fluent. The body-fitted mesh around the cylinder surface is so created that the grid resolution is comparable to the LB simulation setup of the problem. The numerical setup comprises SIMPLE algorithm as the pressure-velocity coupling scheme while maintaining a second-order upwind scheme for spatial discretization of the momentum and energy equations. The convergence criteria is set as 10^{-6} for all the equations. The mentioned discretization scheme is followed while using the Ansys® Fluent in all test cases appearing in the subsequent chapters of this thesis.

Fig. 4.28 shows the variation of surface Nu over the cylinder's surface, where the smooth variation of the Nu using Ansys® Fluent can be attributed to the use of body-fitted mesh around the cylinder. However, several peaks and valleys in thermal-PSC data is evident due to the spurious signals pertaining to the diffuse-interface treatment and subsequent smoothening of these signals. Despite this limitation, which is inevitable in any diffuse-interface IB solver, thermal-PSC shows an excellent agreement of the surface Nu over the cylinder in comparison to that obtained using Ansys® Fluent.

4.3.6 Sedimentation of a cold particle in a heated channel

So far, the capability of the thermal-PSC models for simulating natural, forced, and mixed convection problems, including both stationary and imposed motion problems,

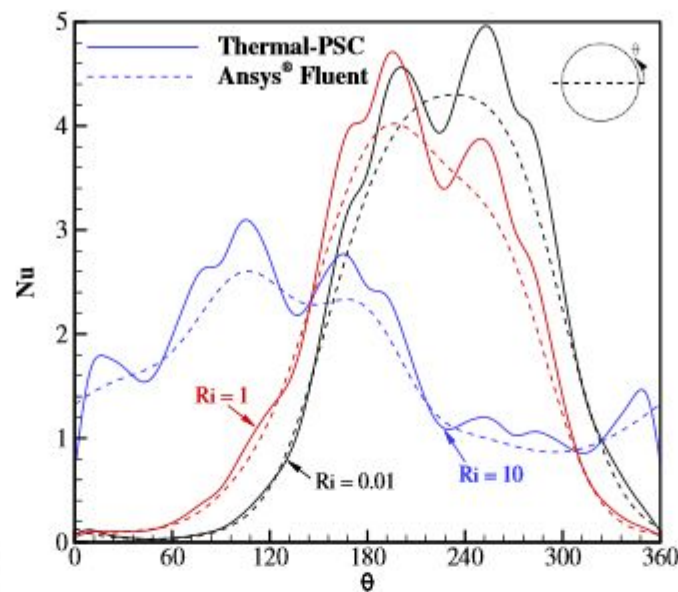


Figure 4.28: Comparison of local Nusselt number over cylinder surface with Ansys® Fluent at various Richardson number.

has been investigated. Now it is intended to put the solver to test its efficacy and robustness when subjected to a complex induced motion scenario, including heat transfer phenomena. In this section, the sedimentation of a constant temperature cold particle is examined in a long-wall bounded heated channel using various thermal-PSC models. This problem involves complex mechanisms between forced convection, natural convection, and the strong wall confinement effect, and thus it's a good selection to validate the solver. This problem was first investigated by Gan et al. [117] using the Arbitrary Lagrangian-Eulerian method (ALE), where the particle is set initially at the vertical center line of the channel and allowed to fall in the channel freely. Based on the evolution of the particle's lateral equilibrium position and different wake structures behind the particle, they classified five flow regimes according to different Grashof numbers (Gr). Subsequently, Yu et al. [119] investigated the problem using the fictitious domain method by placing the initial location of the particle one radius offset from the vertical centerline. The reason for such modification, in contrast to the case of Gan et al. [117] is attributed to the fact that some cases where a particle's trajectory moves away from the domain centerline are not deterministic due to random numerical disturbances. In later years, this problem is revisited by other researchers [63, 67, 73].

As shown in Fig. 4.29, the dimensions of Eshghinejadfard and Thévenin [67] and Suzuki et al. [73] are followed so that direct comparison can be done. Circular cylinder of diameter d is placed at location $(X_c, Y_c) = (1.5d, 4d)$ in a long channel of size $4d \times 40d$. The particle to fluid density ratio ($\rho_r = \rho_p/\rho_f$) is set to 1.00232

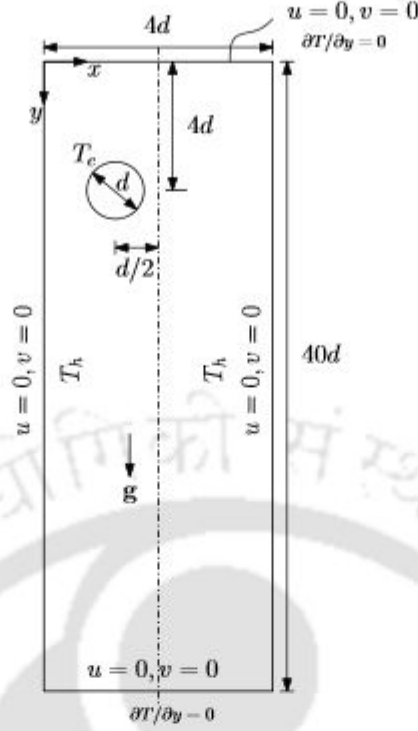


Figure 4.29: Schematic showing the computational domain and boundary conditions of cold particle sedimentation in a heated channel

and is allowed to fall freely under the action of gravity. The buoyancy force due to thermal expansion is evaluated using Boussinesq approximation [Eq. (2.12)], where the reference temperature (T_0) is taken as T_h in the present problem. The cylinder is maintained at constant cold temperature ($T_c = 0$) whereas the side walls and the initial temperature of the fluid are set to hot temperature condition at $T_h = 1$. The channel initially contains a quiescent medium, and all channel walls and cylinder boundaries are subjected to no-slip boundary conditions. The particle motion and its associated dynamics using PSC methodology are elaborated in detail in the preceding Chapter 3. The governing non-dimensional parameters for the problem are: Reynolds number ($Re_{ref} = U_{ref}d/\nu_f$), Prandtl number ($Pr = \nu_f/\chi_f$) and Grashof number ($Gr = \mathbf{g}\beta\Delta Td^3/\nu_f^2$) where $\Delta T = T_h - T_c$. The reference velocity (U_{ref}) based on reference Reynolds number (Re_{ref}) is defined as

$$U_{ref} = \sqrt{\pi \left(\frac{d}{2}\right) \mathbf{g}(\rho_r - 1)} \quad (4.10)$$

In the present simulation, 60 number of lattice nodes are set across the diameter of the particle, $\tau_f = 0.62$, and $Pr = 0.7$, which leads to $\tau_{g,f} = 0.586$ and LB level acceleration due to gravity, $\mathbf{g} = 3.334 \times 10^{-3}$ [using Eq. (4.10)]. The Gr is varied ($Gr = 0, 564, 2000, 2500, 4500$) corresponding to different flow regimes classified by

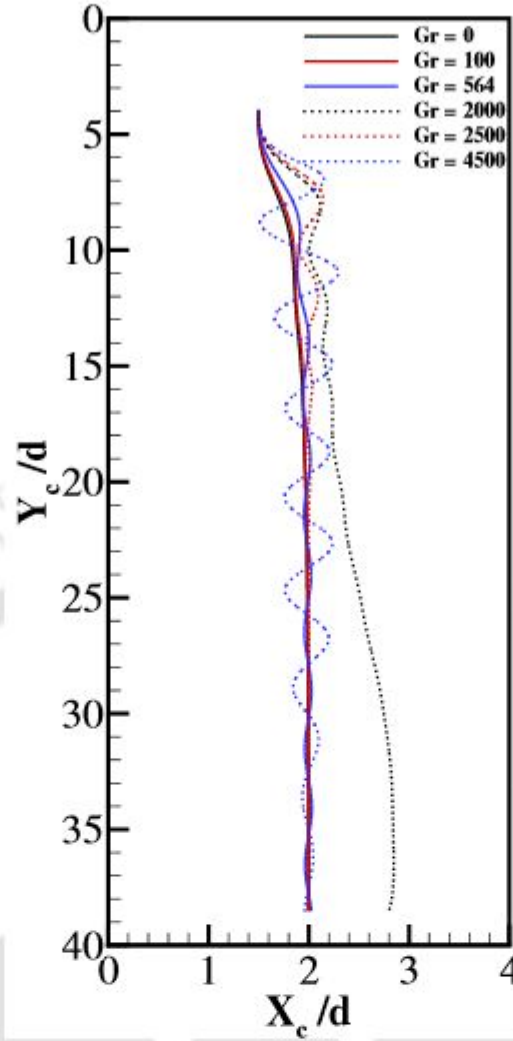


Figure 4.30: Trajectory of particle's center of mass for different Grashof numbers.

Gan et al. [117]. As pointed out by Yu et al. [119], Gan et al. [117] did not provide sufficient information to calculate the reference Reynolds number whereas they mentioned Re based on terminal settling velocity $Re_T = 21$ at $Gr = 0$. Yu et al. [119] found $Re_{ref} = 40.5$ corresponding to $Re_T = 21.2$ at $Gr = 0$ which is in well agreement with Gan et al. [117] result. Thus, the present simulations also utilize $Re_{ref} = 40.5$. It is to be mentioned here that the terminal Reynolds number (Re_T) corresponding to the isothermal case (i.e., $Gr = 0$) using the thermal-PSC model is 20.98. It is in well agreement and within 1.04% relative error with respect to that obtained by Gan et al. [117] and Yu et al. [119] as 21.0 and 21.20, respectively. Different flow regimes (as classified by Gan et al. [117]) based on the particle's lateral equilibrium position and wake structure behind the particle at different Grashof numbers are tabulated in the Table 4.1.

Fig. 4.30 and 4.31 shows trajectory of the particle's center of mass and instantaneous vorticity contours corresponding to different flow regimes mentioned above.

Table 4.1: Classification of different flow regimes during cold particle sedimentation at different Grashof numbers according to Gan et al. [117]

Regime	Particle lateral equilibrium position	Wake structure behind the particle
A ($0 < Gr < 500$)	Settles steadily along vertical centerline	Steady and symmetric vortices
B ($500 < Gr < 810$)	Periodic oscillation about centerline	Vortex shedding occurs
C ($810 < Gr < 2150$)	First experiences oscillating behavior, and then settles steadily close to one of the walls	Vortex shedding absent at steady state
D ($2150 < Gr < 4500$)	Stable equilibrium along channel centerline	Vortex shedding disappears
E ($Gr > 4500$)	Re-emergence of lateral oscillations	Roll-up of shear layers in the wake due to Kelvin-Helmholtz instability

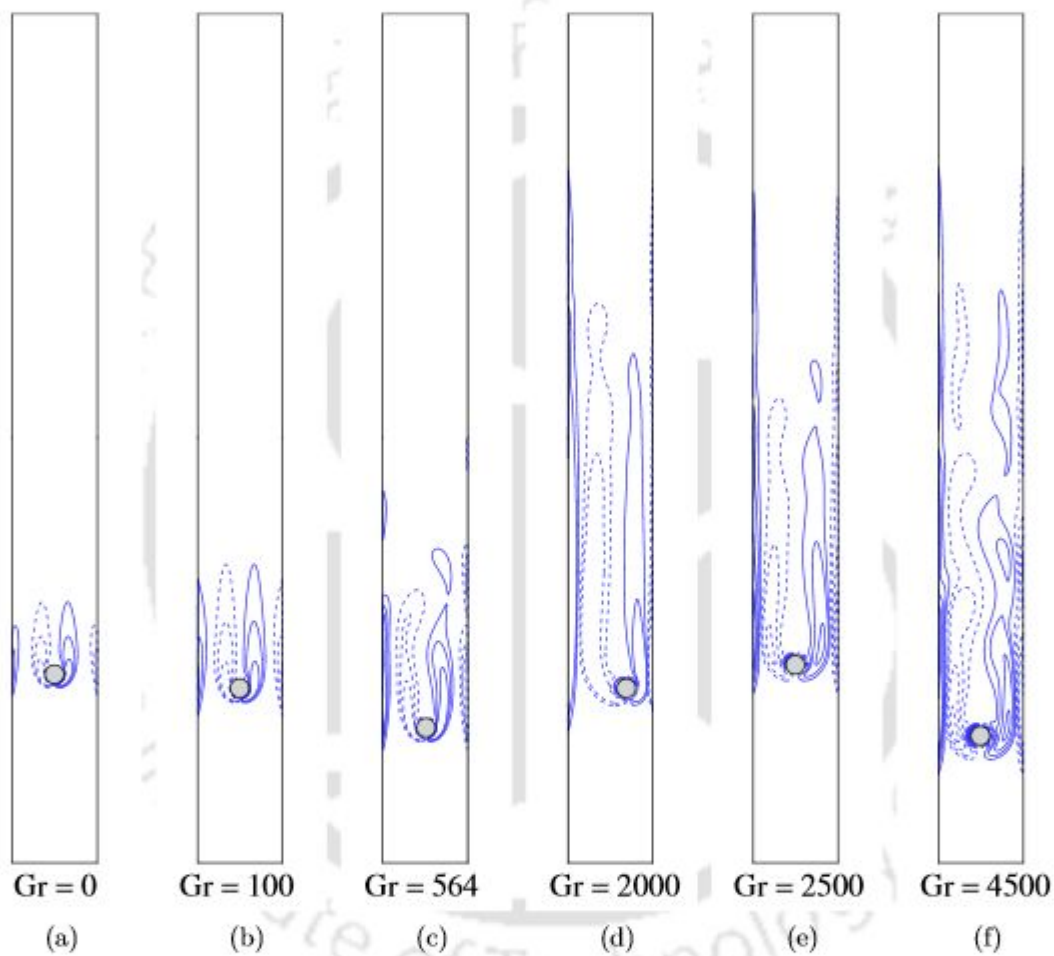


Figure 4.31: Instantaneous vorticity contours of cold particle sedimentation at different Grashof numbers.

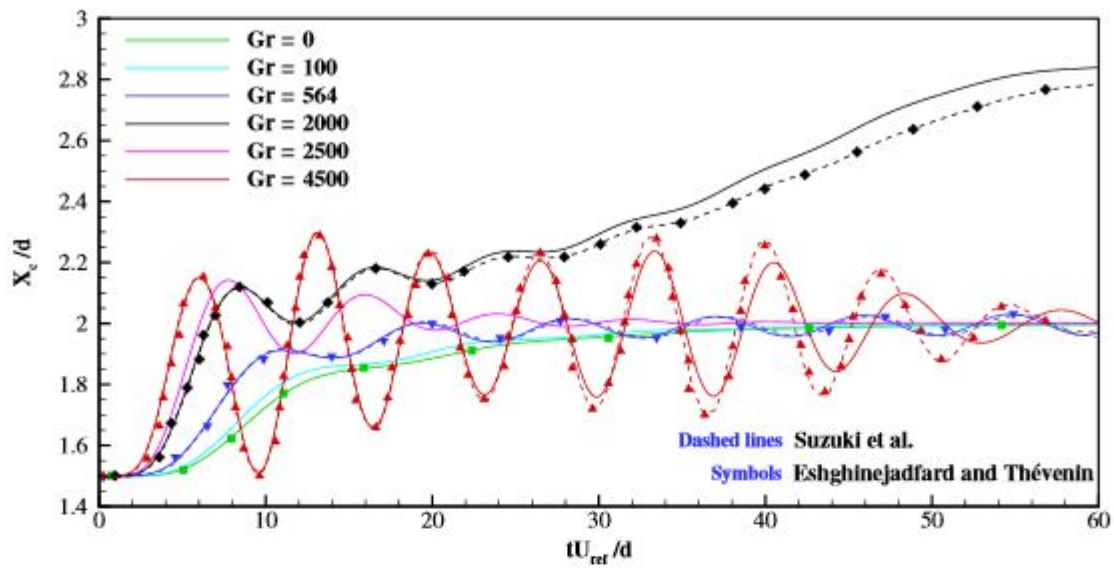


Figure 4.32: Time evolution of particle's lateral position for different Grashof numbers and comparison with Eshghinejadfard and Thévenin [67] and Suzuki et al. [73].

These figures reveal that the present solver re-produced the flow physics in accordance with the flow regimes classified by Gan et al. [117]. Furthermore, Yu et al. [119] reported having observed a new Regime F in contrast to Gan et al. [117] observation at $Gr = 4500$, in which the particle oscillates violently along the centerline and exhibited turbulence-like flow. However, the reason for such discrepancy was not clear to them but attributed the result to the fact that fine mesh is required at far field, too, in order to capture this flow regime. However, the present solver does not reveal any such turbulence-like flow as well as large amplitude oscillations of the particle, although a noticeable larger value is observed at $Gr = 4500$ in accordance with the observation made by Eshghinejadfard and Thévenin [67] and Suzuki et al. [73]. Fig. 4.32 represents comparison of time evolution of particle's lateral trajectories using the thermal-PSC solver with literature [67, 73]. At $Gr = 0$, i.e., the isothermal case, and at $Gr = 564$, the thermal-PSC model exhibits an excellent match in trajectory with respect to that obtained by Eshghinejadfard and Thévenin [67] and Suzuki et al. [73]. Although no data was available in the considered literature [67, 73] for comparison at $Gr = 100$ and 2500 , the trajectory of the particle is in well accordance with the flow physics remarked in Table 4.1. It becomes interesting to note that when the particle starts experiencing oscillations at $Gr = 2000$ and approaches near the wall, where it again experiences high-velocity gradients due to the wall effects, the thermal-PSC model starts deviating from the literature [67, 73] post non-dimensional time $tU_{ref}/d > 30.0$. Subsequently, when the lateral oscillations of the particles re-emerges at $Gr = 4500$, similar deviation is noticed post non-dimensional time $tU_{ref}/d > 30.0$

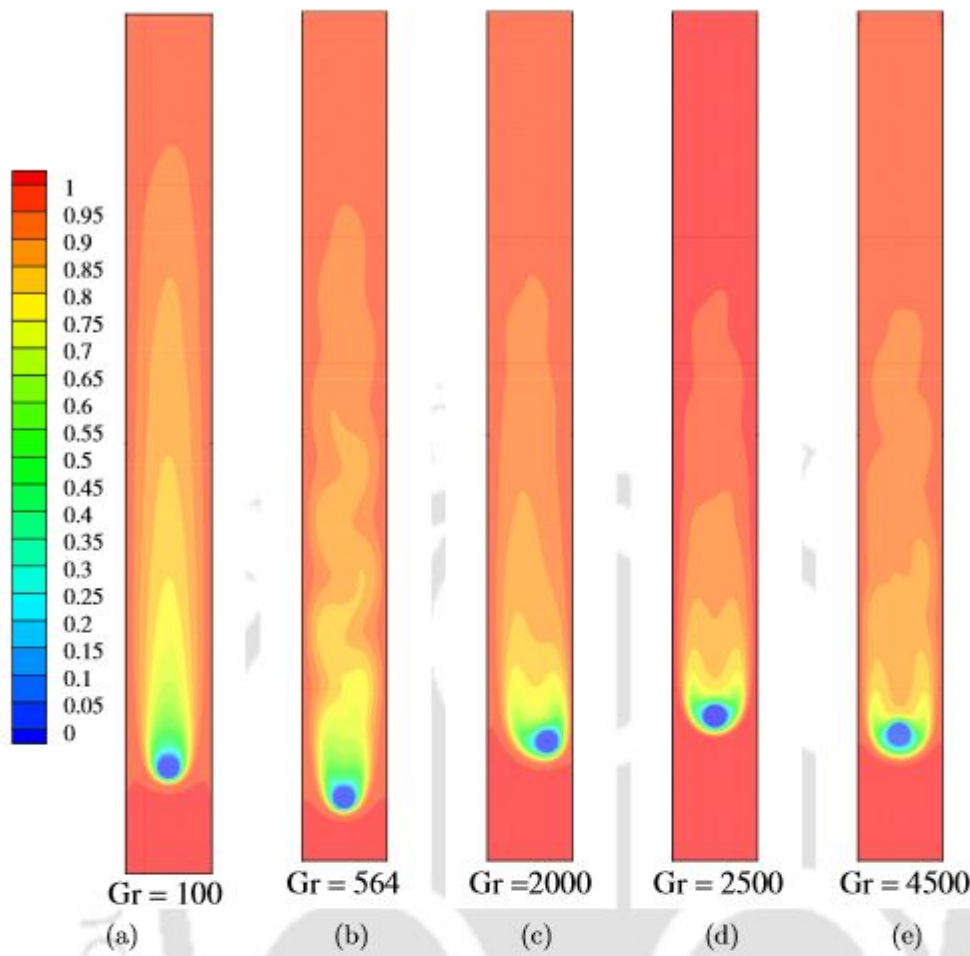


Figure 4.33: Instantaneous temperature contours of cold particle sedimentation at different Grashof numbers.

for both models. Nevertheless, the snapshots of instantaneous temperature contours (Fig. 4.33) at different Grashof numbers using the present solver are in well agreement with that obtained by Suzuki et al. [73] and Eshghinejadfard and Thévenin [67]. In a nutshell, one can conclude that the thermal-PSC model can be reckoned for mixed convection problems involving stationary and moving boundaries.

4.4 Summary

The present chapter deals with an extensive analysis of the Partially Saturated Computational cells (PSC) method for simulating incompressible thermal flows involving forced, free, and mixed convection phenomena, which also encompasses stationary, imposed, and induced motion scenarios. The accuracy study of the algorithm during a moving boundary scenario reveals it to be a first-order accurate method with respect to the grid resolution irrespective of the solid surface being straight or curved. The

thermal-PSC model exhibits more sensitivity towards τ_f in curved boundaries than straight ones. The algorithm is Galilean invariant and exhibits approximately identical local and average Nusselt number variation in moving and stationary reference frames. Furthermore, the algorithm is investigated in terms of the prediction of local heat transfer characteristics in a wide spectrum of benchmark problems. The present model can estimate the local Nusselt number over curved surfaces with better accuracy for forced and mixed convection problems as compared to the free convection problems. This limitation of the model can be worked upon in the future to obtain a better version of the PSC model for natural convection problems. However, with specific advantages and limitations, the present work conclusively demonstrates the efficacy and robustness of the thermal-PSC algorithm for incompressible thermal flows.



CHAPTER 5

COMPARATIVE STUDY OF DIRECT-FORCING IB-LB AND PSC METHODOLOGY

“Theory is good, but mankind has always needed numbers”

- Gretar Tryggvason, *CFD Symposium, 2010*

The present chapter demonstrates a comparative analysis of the Partially Saturated Cells method with respect to a popular IB-LB method in the literature, namely the direct-forcing IB-LB method. The focal point of the analysis targets four facets of numerical appraisal, viz., accuracy, discrete conservation of properties, spurious force oscillations in moving boundary problems, and the Galilean invariance in thermo-fluidic applications. The investigation reveals that PSC and DF-IB-LB methods exhibit a linear decay in velocity and temperature errors, while the pressure error experiences a quadratic declination with respect to grid refinement. In addition, the τ_f sensitivity analysis for velocity, pressure, and temperature errors is presented in this chapter. The discrete conservation study assures that PSC can ensure discrete mass conservation comparable to the DF-IB-LB approach. Furthermore, the spurious force oscillations experienced by the PSC method decay at a rate of 1.67, while the DF-IB-LB approach decays at a rate of 2.48 with grid refinement. Nevertheless, the pressure drag coefficient using the PSC approach reveals lesser spurious fluctuations than the DF-IB-LB method at any instant. The study also reveals that the PSC and the DF-IB-LB approaches are Galilean invariant for hydrodynamic and heat transfer applications. In a nutshell, the

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present investigation endorses that the PSC approach can predict accurate thermo-fluidic characteristics in complex boundary problems comparable to the conventional DF-IB-LB method.

The Chapter 1 of the present thesis highlights that the prominent variants of immersed boundary-lattice Boltzmann methodologies (IB-LB) are penalty-force method [39], direct forcing IB-LB method [40], momentum-exchange based method [42], velocity correction method [43] and partially saturated cells method [45]. The conventional treatment of boundary conditions [7, 120] in LBM instigates spuriousness in hydrodynamic forces at the fluid-particle interface, further necessitating to use of specialized techniques such as the refill-algorithm [34, 121] to mitigate the same. However, the limitations of the conventional LBM can be overcome by coupling Immersed Boundary (IB)-Lattice Boltzmann method (LB) [39, 40]. The author realizes that the DF-IB-LB method is popular and extensively utilized in open literature owing to its simple algorithm and exhibition of comparable accuracy compared to the aforementioned variants of the IB-LB methods. However, the PSC model also exhibits promising efficacy and robustness for simulating incompressible flows past complex moving structures as demonstrated in several articles [50, 51] and Chapter 3 of the present thesis. Thus the motivation behind a comparative analysis of the PSC and the DF-IB-LB method is attributed to the boundary condition implementation of these techniques. While these methods recognize themselves in the class of diffuse-interface IB-LB techniques, the former utilizes a volume fraction-based formulation, and the latter comprises the Eulerian-Lagrangian framework for realizing the solid-fluid interface. The boundary conditions in PSC are implemented by virtue of the solid collision operator incorporated in the evolution equation, whereas the same is achieved through momentum balance at Lagrangian node points in the DF-IB-LB method. While the accuracy of such implementations in PSC can be attributed to the robustness of the solid collision operator, the DF-IB-LB method primarily relies on the distribution techniques used for interpolating flow parameters from Eulerian nodes to the Lagrangian nodes and vice-versa. Hence, the comparative analysis would reveal the viability of the present PSC algorithm as compared to the conventional DF-IB-LB method used by the computational LB community. In the next section, brief mathematical formulations of the DF-IB-LB and DF-IB-TLB methods are presented to enhance the readability of the thesis.

5.1 Direct forcing IB-LB and IB-TLB formulation

The evolution equation for the DF-IB-LB method can be expressed by adding a discrete forcing term (F_i) in the discretized LB governing equation [Eq. (2.1)] as

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i^{BGK}(\mathbf{x}, t) + F_i \Delta t \quad (5.1)$$

The Eq. (5.1) is solved at Eulerian lattice nodes, from where information (in terms of pressure, velocity, temperature, etc.) is interpolated to immersed Lagrangian nodes as shown in Fig. 5.1. Hydrodynamic forces experienced by the body due to its motion and fluid-particle interactions are computed at Lagrangian boundary nodes, which are then suitably re-distributed onto the Eulerian nodes in the fluid regime. The direct forcing term (F_i) in Eq. (5.1) can be expressed as,

$$F_i = \left(1 - \frac{1}{2\tau_f}\right) \omega_i \left(\frac{\mathbf{c}_i - \mathbf{u}}{c_s^2} + \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^4} \mathbf{c}_i \right) \cdot \mathbf{F}_b \quad (5.2)$$

where $\mathbf{F}_b(\mathbf{x}, t)$ is the fluid body force density. Once the non-forced velocity at the Lagrangian nodes is obtained, one can calculate the particle boundary force density at the m^{th} Lagrangian node at position $\mathbf{X}_m$ using Eq. (5.3).

$$\mathbf{F}(\mathbf{X}_m, t) = \frac{2}{\Delta t} [\mathbf{U}^d(\mathbf{X}_m, t) - \mathbf{U}^*(\mathbf{X}_m, t)] \quad (5.3)$$

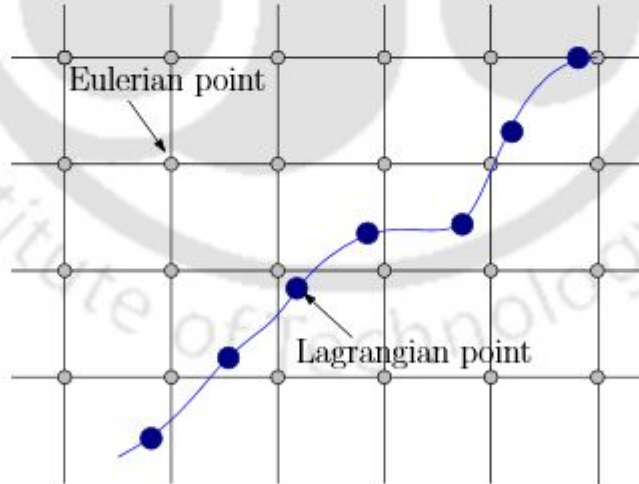


Figure 5.1: Illustration of the Immersed Boundary method. The Lagrangian points represent the boundary and the intersection of the mesh lines represent the Eulerian fluid points. This figure is identical to Fig. 1.5. It is put here to enhance the readability of the chapter.

where $\mathbf{U}^d$ is the desired velocity at the Lagrangian point, and $\mathbf{U}^*$ is the interpolated fluid velocity at the Lagrangian node obtained from Eq. (5.4).

$$\mathbf{U}^*(\mathbf{X}_m, t) = \sum_{i,j} \mathbf{u}(\mathbf{x}, t) \delta_h(\mathbf{x} - \mathbf{X}_m) h^2 \quad (5.4)$$

The non-forced fluid velocity $\mathbf{u}(\mathbf{x}, t)$ at the Eulerian nodes is obtained using Eq. (2.4b), and the particle boundary force density $\mathbf{F}(\mathbf{X}_m, t)$ is spread to neighboring Eulerian nodes as

$$\mathbf{F}_b(\mathbf{x}, t) = \sum_m \mathbf{F}(\mathbf{X}_m, t) \delta_h(\mathbf{x} - \mathbf{X}_m) \Delta s \quad (5.5)$$

where Δs is the arc length. $\delta_h(\mathbf{x}_{ij} - \mathbf{X}_m)$ is a continuous kernel function which approximates the Dirac Delta function as

$$\delta_h(\mathbf{x} - \mathbf{X}_m) = \frac{1}{h^2} \phi\left(\frac{x - X_m}{h}\right) \phi\left(\frac{y - Y_m}{h}\right) \quad (5.6)$$

where h is mesh spacing. Δs should be adopted such that it averts mass-leakage and ensures no-slip boundary condition. Peskin [122] proposed $\Delta s \leq h/2$ and Cheng et al. [123] suggested $\Delta s < h$ for obtaining accurate results. In the present study, number of Lagrangian nodes over the particle's surface is adopted as 1.2 times (C/h), where C is the circumference of the particle. It leads to $\Delta s \approx 0.83h$. Finally, the velocity is updated according to Eq. (5.7) that reads,

$$\rho_0 \mathbf{u}(\mathbf{x}, t) = \sum_i \mathbf{c}_i f_i + 0.5 \mathbf{F}_b(\mathbf{x}, t) \Delta t \quad (5.7)$$

The present work considers a two-point stencil kernel function which is expressed as

$$\phi(r) = \begin{cases} 1 - |r|, & |r| \leq 1 \\ 0, & |r| > 1 \end{cases} \quad (5.8)$$

The evolution equation for the direct-forcing immersed-boundary thermal lattice-Boltzmann (DF-IB-TLB) method applicable for thermal flows can be expressed by adding a heat source term [65] in each lattice direction in the STLBE [Eq. (2.7)] as

$$g_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = g_i(\mathbf{x}, t) + \frac{\Delta t}{\tau_{g,f}} [g_i^{eq}(\mathbf{x}, t) - g_i(\mathbf{x}, t)] + \left(1 - \frac{1}{2\tau_{g,f}}\right) w_i Q_b \Delta t \quad (5.9)$$

Here, Q_b represents the heat source term at each Eulerian node. The heat source term on each Lagrangian node (m) can be expressed as

$$Q(\mathbf{X}_m, t) = \frac{2}{\Delta t} [T^d(\mathbf{X}_m, t) - T^*(\mathbf{X}_m, t)] \quad (5.10)$$

The $T^d(\mathbf{X}_m, t)$ signifies the desired temperature, and the $T^*(\mathbf{X}_m, t)$ refers to the no-heating temperature on each Lagrangian node which is obtained by interpolating temperature from the neighbouring Eulerian nodes.

$$T^*(\mathbf{X}_m, t) = \sum_{i,j} T(\mathbf{x}, t) \delta_h(\mathbf{x} - \mathbf{X}_m) h^2 \quad (5.11)$$

$T(\mathbf{x}, t)$ at Eulerian node is evaluated using the Eq. (2.11). The heat source term at m^{th} Lagrangian node obtained using Eq. (5.10) can be spread to the neighbouring Eulerian nodes to determine the Q_b following the Eq. (5.12).

$$Q_b(\mathbf{x}, t) = \sum_m Q(\mathbf{X}_m, t) \delta_h(\mathbf{x} - \mathbf{X}_m) \Delta s \quad (5.12)$$

Finally, the temperature of each Eulerian node is updated using Eq. (5.13).

$$T(\mathbf{x}, t) = \sum_i g_i(\mathbf{x}, t) + 0.5 Q_b(\mathbf{x}, t) \Delta t \quad (5.13)$$

Detailed computational steps for numerical simulations using the DF-IB-LB and DF-IB-TLB methods are illustrated in Algorithm 3.

5.2 Accuracy study

The Sections 3.1.2 and 4.1.2 illustrate that the PSC model exhibits first-order spatial convergence in velocity and temperature errors while maintains a second-order convergence in pressure errors with respect to grid refinement. In addition, the model also reveals a dependence on τ_f while evaluating these errors. In light of these facts, the present section compares the order of accuracy of the PSC algorithm for hydrodynamic and thermal flows with respect to the DF-IB-LB and DF-IB-TLB methods, respectively. The popular Taylor-Couette problem and the cylindrical-Couette flow are chosen for the investigations primarily because of the involvement of curved surfaces which are not aligned with the underlying Cartesian grid. In addition to evaluating spatial order of accuracy, the algorithms' dependency on the selection of relaxation time (τ_f) is also presented.

5.2.1 Taylor-Couette problem

The well-known Taylor-Couette problem is a classical test case often used to establish the accuracy of moving boundary problems as it constitutes both stationary and moving complex boundaries. The fact that this flow field has an exact analytical so-

Algorithm 3: Computational steps for DF-IB-LB and DF-IB-TLB approaches.

```

Grid generation;
Initialization;
for each time step  $t$  do
    Obtain direct-forcing term in each lattice direction using Eq. (5.2). This
    force would also include thermal forces during natural and mixed
    convection problems;
    Apply DF-IB-LB governing equations via collision and streaming steps
    [Eq. (5.1)];
    Apply boundary condition at domain boundaries following Zou and He
    [11];
    Evaluate macroscopic variables using Eqns. (2.4a) and (2.4b);
    Interpolate velocities from Eulerian nodes to the Lagrangian nodes using
    Eq. (5.4) ;
    Compute hydrodynamic forces at Lagrangian nodes using Eq. (5.3);
    Spread the Lagrangian forces to neighbouring Eulerian nodes using Eq.
    (5.5);
    Update the Eulerian velocities using Eq. (5.7). The correction is
    constituted using the hydrodynamic forces evaluated in Eq. (5.5);
    Apply DF-IB-TLB governing equations via collision and streaming steps
    [Eq. (5.9)];
    Apply thermal boundary conditions at domain boundaries following Liu et
    al. [86];
    Evaluate macroscopic temperature ( $T$ ) using Eq. (2.11) ;
    Interpolate temperature from Eulerian nodes to the Lagrangian nodes
    using Eq. (5.11) ;
    Compute heat source term at Lagrangian nodes using Eq. (5.10);
    Spread the computed direct-heating term from Lagrangian nodes to the
    neighbouring Eulerian nodes using Eq. (5.12);
    Update the temperature of Eulerian nodes using Eq. (5.13);
    Obtain thermal force following the Boussinesq approximation using Eq.
    (2.12);
    Update the Eulerian velocities using Eq. (2.15). The correction is
    constituted using the thermal forces evaluated in Eq. (2.12);
    Obtain total hydrodynamic forces as  $\mathbf{F} = -\sum_m \mathbf{F}(\mathbf{X}_m, t)\Delta s$ ;
    Calculate translational [Eq. (2.26)] and angular velocities of the particle
    [Eq. (2.27)];
    Update particle location  $\mathbf{X}_c$  using Eq. (2.28a);
    Obtain desired particle velocity  $\mathbf{U}_p$  on the surface of the particle using Eq.
    (2.28b)
end

```

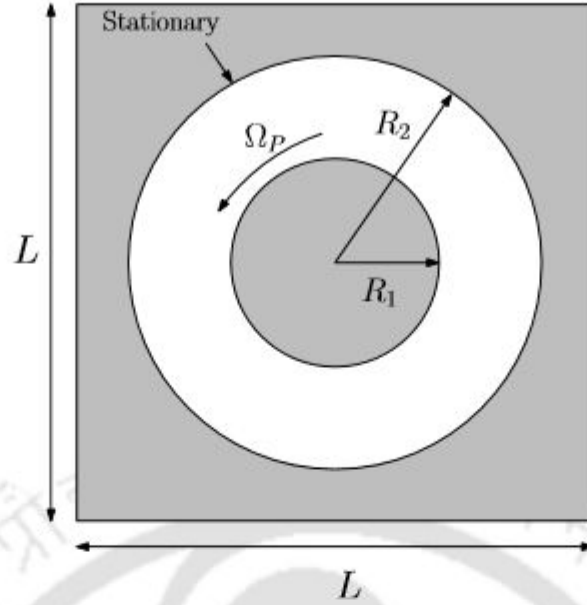


Figure 5.2: Computational domain for Taylor-Couette problem. This figure is identical to Fig. 3.2. It is put here to enhance the readability of the chapter.

lution [Eqns. (3.2)] makes it an ideal validation case for spatial accuracy studies. To facilitate the study, two concentric cylinders of radii $R_1 = 0.2L$ and $R_2 = 0.4L$ are immersed into a square computational domain of side $L = 1$ as represented in Fig. 5.2. The inner cylinder is subjected to a constant angular velocity $\Omega_p = U/R_1$ while the outer cylinder is static. The computational domain boundaries are prescribed as no-slip walls, and impermeable cylinder surfaces should restrict the flow only inside the annular region. Four different grid resolutions are considered to facilitate the order of accuracy analysis, viz. $\Delta x = L/40, L/80, L/160$, and $L/320$, while maintaining identical $Re = U(2R_1)/\nu_f = 10$ and convergence criterion of 10^{-8} for steady state computations. The rates of velocity and pressure error decay with respect to the grid refinement at $\tau_f=1.0$ are depicted in Fig. 5.3. Both L_∞ and L_2 error norms for velocity errors decay approximately linearly with grid refinement. The average experimental order of convergence (EOC) in (L_∞ and L_2) velocity error norms are (0.956, 1.058) and (0.918, 0.978) using the PSC and DF-IB-LB methods, respectively. The first-order decline in velocity errors can be attributed to the presence of discontinuity in velocity gradients on the fluid-solid interface of IB-LB methods [44, 66, 124]. However, the pressure error exhibits nearly quadratic decay with grid refinement having an average EOC around 1.7 for both the methodologies, independent of the value of τ_f .

In order to establish the dependence of relaxation time (τ_f) on error norms of the DF-IB-LB method, the grid resolution is fixed at $\Delta x = L/80$ and the τ_f is varied from 0.6 to 2.0. Figure 5.4 reveals that velocity error norms using the DF-IB-LB method decrease with an increase in τ_f until $\tau_f = 1.5$ beyond which they exhibit an increasing

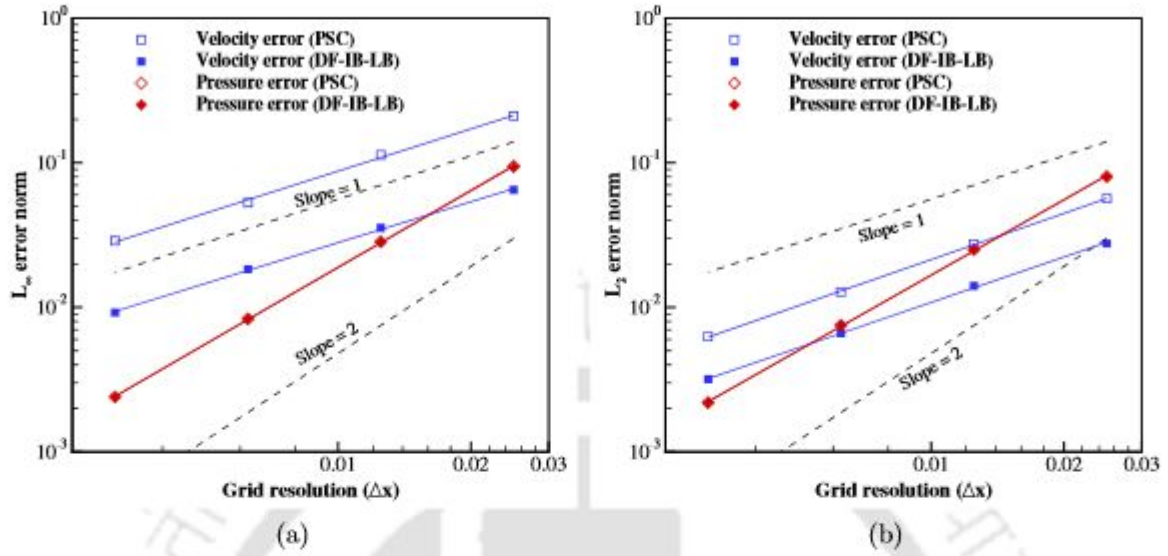


Figure 5.3: Comparison of the velocity and pressure error norms using PSC and DF-IB-LB methods with respect to grid resolution (a) L_∞ error and (b) L_2 error.

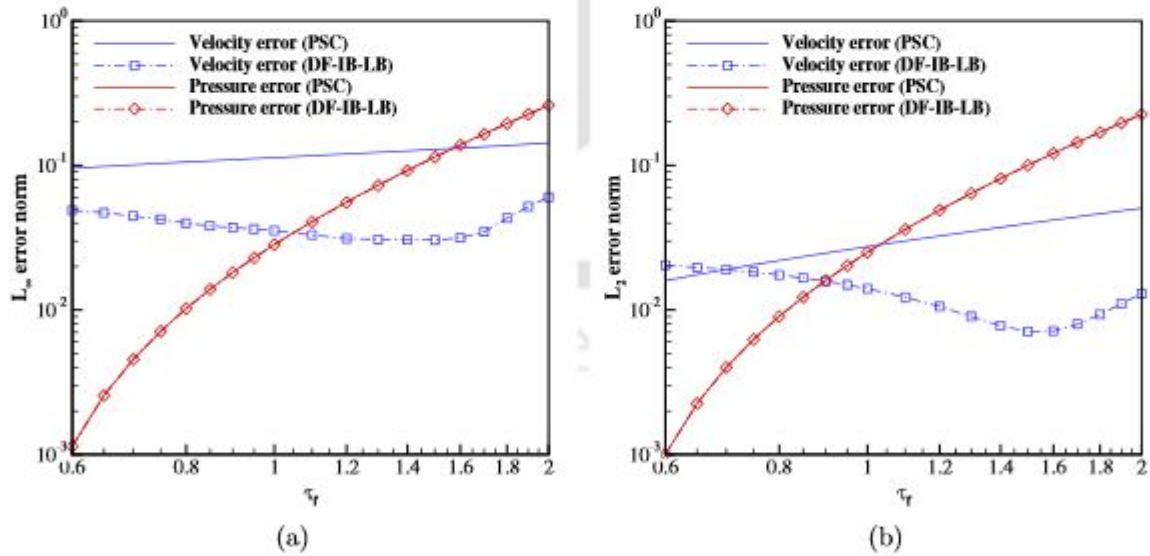


Figure 5.4: Comparison of the velocity and pressure error norms using PSC and DF-IB-LB methods with respect to varying τ_f for Taylor-Couette problem. (a) L_∞ error and (b) L_2 error.

Table 5.1: Comparison of relative % error of the torque using PSC and DF-IB-LB methods with respect to the analytical torque ($T^{ana} = -2.3271$) for different grid resolutions.

Δx	PSC		DF-IB-LB	
	Torque	% error	Torque	% error
0.025	-2.0299	12.77	-2.5430	9.276
0.0125	-2.1702	6.741	-2.4205	4.013
0.00625	-2.2470	3.442	-2.3743	2.029
0.003125	-2.2871	1.719	-2.3514	1.044

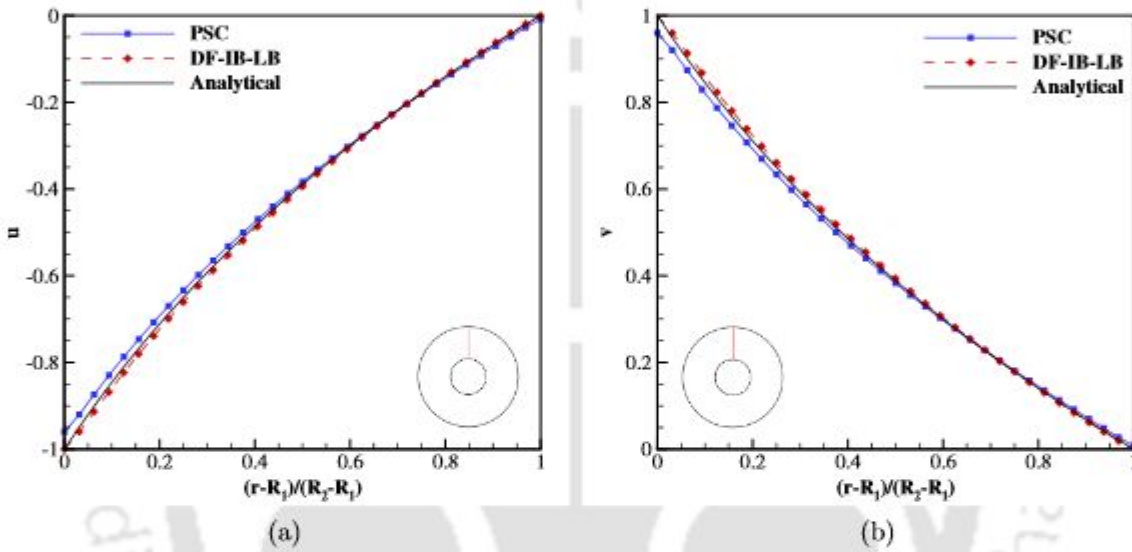


Figure 5.5: Comparison of numerical and analytical solutions of velocity profiles using PSC and DF-IB-LB methods. (a) u-velocity profile at $x = 0$ and (b) v-velocity at $y = 0$.

trend. On the contrary, velocity error norms using PSC exhibit an increase in error with the increase in τ_f and possess a higher magnitude of errors as compared to that obtained using DF-IB-LB. The pressure error norms, however, exhibit a monotonic increase in magnitude with the increasing τ_f and carry the identical magnitude of errors for both approaches. Table 5.1 shows the relative torque error of PSC and DF-IB-LB methods reduces with grid refinement at a rate of approximately first order. In addition to it, the comparison of velocity profiles using PSC and DF-IB-LB methods in Fig. 5.5 reveals that both the methods exhibit an excellent degree of conformity with the exact velocity profiles. However, a deviation in the prediction of the velocity adjacent to the moving cylinder is observed for the PSC approach. This minute aberration can be attributed to its volume fraction-based diffusive algorithm for implementing the boundary conditions, unlike the presence of Lagrangian points on the exact curved surfaces for the same act in the DF-IB-LB approach. Nevertheless, the

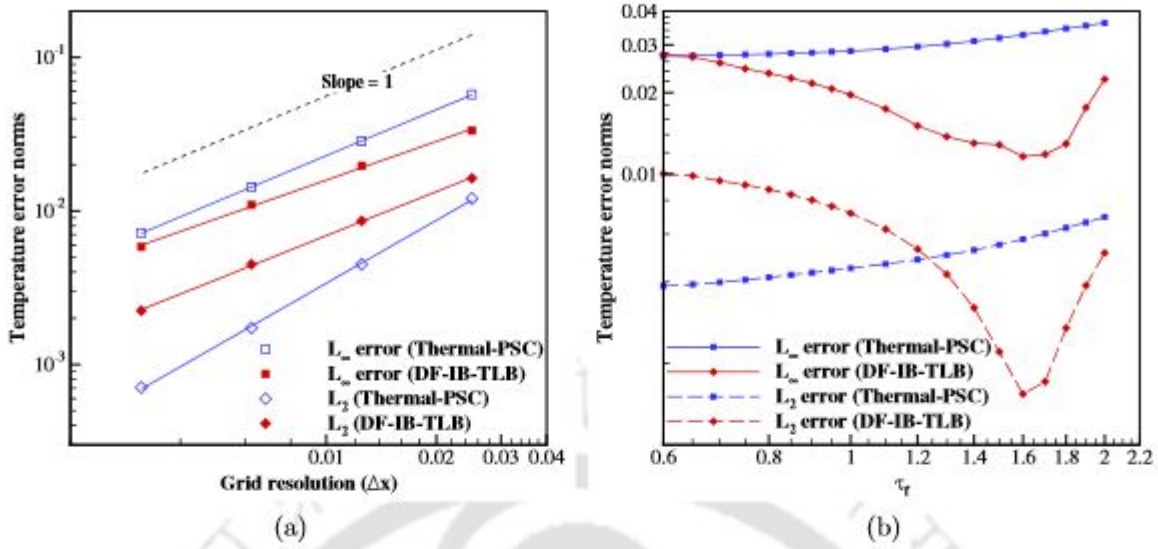


Figure 5.6: Comparison of the temperature error norms using PSC and DF-IB-TLB methods with respect to (a) grid resolution (Δx) and (b) variation in τ_f .

present investigation demonstrates that the PSC algorithm is comparable to the conventional DF-IB-LB method for accurately predicting hydrodynamical characteristics across complex geometries.

5.2.2 Cylindrical thermal-Couette flow

The present subsection examines the preceding problem subjected to Dirichlet thermal boundary conditions, which will facilitate a direct comparison between DF-IB-TLB and thermal-PSC methodologies. The inner cylinder is prescribed a higher temperature T_1 while the outer cylinder is set to a lower temperature T_2 as illustrated in Fig. 4.4. The hydrodynamic boundary conditions and simulation parameters are defined identically to that mentioned in the previous Section 5.2.1. The non-dimensional parameters for this problem are defined and set as Reynolds number ($Re = (R_1 \Omega_P)(2R_1)/\nu_f = 10$) and Prandtl number ($Pr = \nu_f/\chi_f = 0.73$). The analytical solution to the temperature field is expressed in Eq. (4.6) while the convergence criterion for steady state computations is set to 10^{-8} .

Fig. 5.6a reveals that both PSC and DF-IB-TLB approaches decay approximately linearly with grid refinement in L_∞ and L_2 temperature error norms. The DF-IB-TLB method experiences a lesser magnitude of L_∞ error than the PSC method. However, the rate of decay of the error using the PSC and DF-IB-TLB methods is 0.99 and 0.84, respectively. Furthermore, the PSC method exhibits a lesser magnitude of L_2 errors than the DF-IB-TLB approach. The slope of the decay experienced by PSC and DF-IB-LB methods in a log-log plot of the temperature error versus the grid resolution

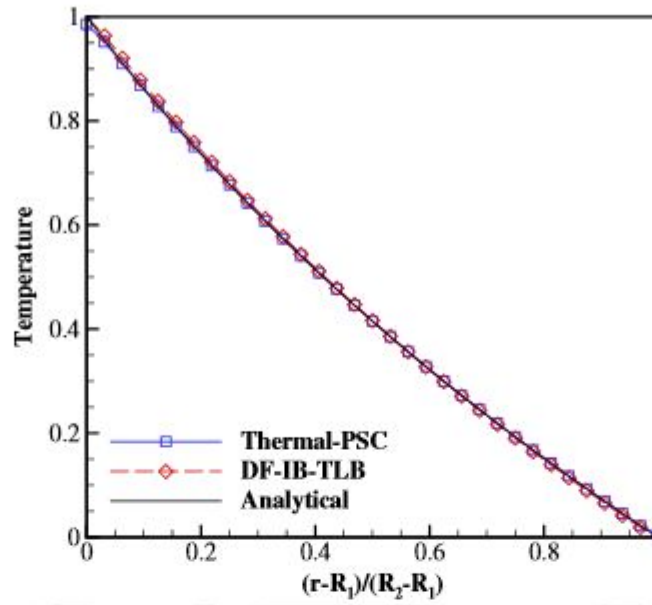


Figure 5.7: Comparison of numerical and analytical solutions of temperature profiles using PSC and DF-IB-TLB methods.

is 1.36 and 0.95, respectively. In addition to it, the τ_f sensitivity test at a fixed grid resolution of $\Delta x = L/80$ illustrated in Fig. 5.6b reveals that the L_∞ and L_2 temperature error norms degrade until $\tau_f = 1.6$ using the DF-IB-TLB approach. However, the PSC approach experiences increased errors with the increase in relaxation time. It can also be observed that the magnitude of L_2 error obtained using the PSC method is lower than that obtained by DF-IB-TLB until $\tau_f = 1.2$. Furthermore, comparing temperature profiles using PSC and DF-IB-TLB methods with respect to the analytical temperature field reveals an excellent agreement and is depicted in Fig. 5.7. Hence, one can conclude from the investigations performed in this section that thermal-PSC yields comparable heat transfer characteristics until relaxation time $\tau_f \leq 1.2$.

5.3 Discrete conservation study

The appraisal of discrete conservation of properties is an important aspect pertaining to the IB-LB method. Yin et al. [93] showed that the artificial treatment of local mass conservation at fluid-solid interface is extraneous in conventional LB boundary condition schemes and could pollute the accuracy of solution in fluid-structure interaction problems. The global mass flux error in simulation using the PSC and DF-IB-LB methods on curved boundary problems is examined, and it reveals that they remain at acceptable levels despite any ancillary treatment at the solid-fluid interface. The investigation is facilitated by considering a flow through a curved channel which is immersed into the underlying regular Cartesian mesh in a computational domain of

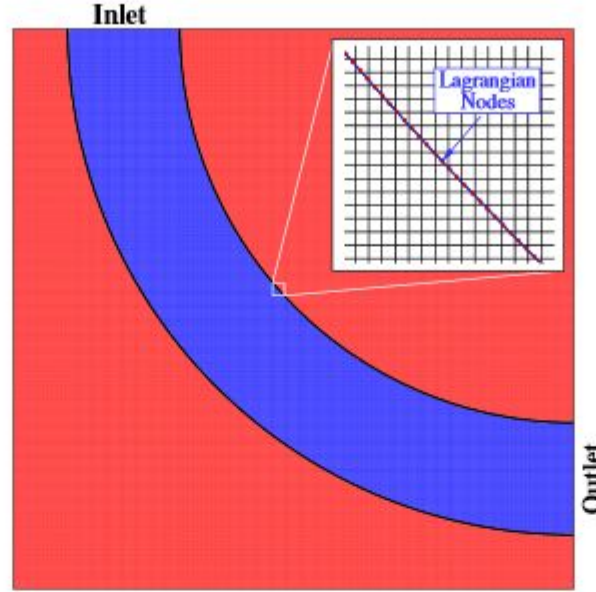


Figure 5.8: Schematic representation of the computational domain with a flow through curved channel.

size $L \times L$. The schematic of the problem is illustrated in Fig. 5.8 and detailed in Section 3.2 of the present thesis.

Figure 5.9 reveals that the local maximum divergence over the entire computational domain is confined to the order of 10^{-4} for both PSC and DF-IB-LB methods, which is an acceptable mass conservation error in most numerical setups. Moreover, the PSC method experiences lower local maximum divergence than the DF-IB-LB method during the course of its iterations. It must also be emphasized that although the lattice-Boltzmann equation recovers Navier-Stokes' equation in the incompressible limit, density cannot be kept constant in LB simulations as otherwise, the pressure changes cannot be captured. Hence, it is necessary to analyze the maximum density fluctuations in the present simulations. The mass flux errors and the maximum density fluctuations using the DF-IB-LB and PSC methods for a fixed value of $\tau_f = 0.6$ and different grid resolutions are summarized in Table 5.2. It is fairly evident from the table that the mass flux errors and the maximum density fluctuations decay with grid refinement for both methodologies considered here. The magnitude of mass flux error in the DF-IB-LB method is two decades lesser than the PSC approach in finer grids. However, the PSC method experiences lesser density fluctuations than the DF-IB-LB method owing to its locality of solid collision operator in the evolution equation. The fact that they decay with grid refinement affirms that the PSC and DF-IB-LB approaches are discretely conservative in the limit of lattice size approaching zero. The next quest of the investigation extends towards examining the effect of relaxation time (τ_f) in discrete conservation of properties. To facilitate the study, simulations are

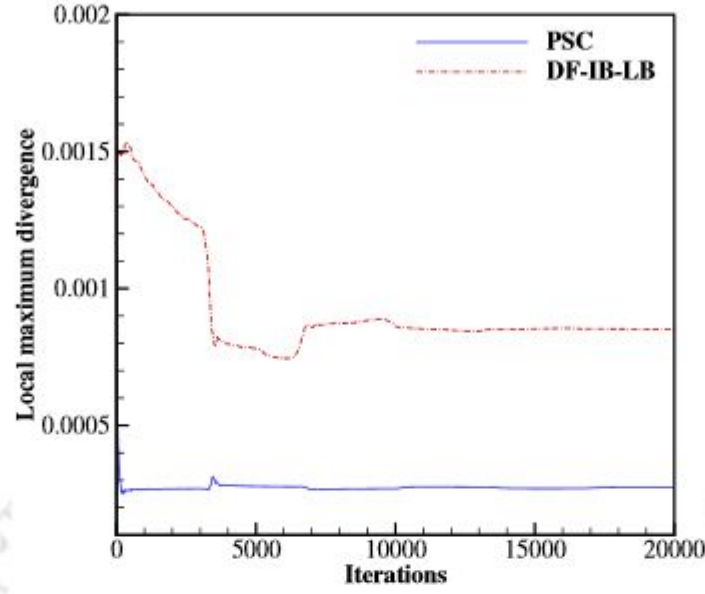


Figure 5.9: Time history of local maximum divergence in flow through curved channel using PSC and DF-IB-LB methods.

Table 5.2: Comparison of mass flux defect and maximum density fluctuation for varying grid and τ_f using PSC and DF-IB-LB

		Mass flux defect $ \dot{m}_{in} - \dot{m}_{out} $	Maximum density fluctuations $(\Delta\rho)_{max}$
Variable grid resolution ($L \times L$) for $\tau_f = 0.6$			
250×250	PSC	1.75×10^{-3}	1.98×10^{-3}
	DF-IB-LB	1.67×10^{-4}	4.28×10^{-3}
500×500	PSC	1.34×10^{-3}	7.75×10^{-4}
	DF-IB-LB	4.47×10^{-5}	1.95×10^{-3}
750×750	PSC	1.00×10^{-3}	4.68×10^{-4}
	DF-IB-LB	1.82×10^{-5}	1.25×10^{-3}
Variable relaxation time (τ_f) for grid resolution of 500×500			
$\tau_f = 0.6$	PSC	1.34×10^{-3}	7.75×10^{-4}
	DF-IB-LB	4.47×10^{-5}	1.95×10^{-3}
$\tau_f = 0.7$	PSC	2.45×10^{-3}	2.69×10^{-3}
	DF-IB-LB	3.42×10^{-4}	4.10×10^{-3}
$\tau_f = 0.8$	PSC	2.20×10^{-3}	5.92×10^{-3}
	DF-IB-LB	1.11×10^{-3}	7.28×10^{-3}
$\tau_f = 0.9$	PSC	1.90×10^{-5}	1.03×10^{-2}
	DF-IB-LB	2.57×10^{-3}	1.11×10^{-2}
$\tau_f = 1.0$	PSC	5.00×10^{-3}	1.56×10^{-2}
	DF-IB-LB	4.89×10^{-3}	1.54×10^{-2}

performed at a fixed grid resolution of $L = 500$ while varying the relaxation time. It is evident from Table 5.2 that the mass flux error increases with τ_f in both PSC and DF-IB-LB methods; however, a local minimum is observed using PSC at $\tau_f = 0.9$. The maximum density fluctuations increase with an increase in τ_f irrespective of the PSC or DF-IB-LB method. Moreover, not shown herein, negligible velocity magnitudes are observed outside the flow domain using both approaches in the vicinity of the curved boundaries, indicative that the no-slip boundary condition is approximately enforced despite the channel boundaries being non-aligned to the underlying Cartesian mesh. This study endorses that the PSC approach can guarantee approximate discrete mass conservation as comparable to the DF-IB-LB methodology.

5.4 Spurious force oscillations

Spurious force oscillations (SFOs) in temporal histories of force coefficients are a major issue pertaining to moving boundary problems. While a body is in motion, the underlying lattice nodes experience a change in identity due to the birth and death of solid-fluid nodes. This identity transformation is often neither continuous nor smooth and can be attributed as the primary cause of SFOs. Kang [100] reported the presence of SFO in force signals for sharp-interface IB-LB schemes and mitigated the same by using standard smoothing or FFT filtering techniques. Although there were no specific comments on SFOs in the direct forcing approach in their studies, it was reported that the approach led to over-prediction of the surface force coefficients. Several other studies [44, 47] have reported the presence of SFOs in the IB-LB methods, but the quantitative comparison of these oscillations as a function of grid resolution for PSC and DF-IB-LB methods are presented in this work.

To facilitate this study, a circular cylinder of diameter d is subjected to an oscillatory motion within an initially quiescent computational domain of size $4d \times 4d$. The simulation parameters and boundary conditions are set identical to those in Seo and Mittal [95] and previously demonstrated in Section 3.3 of this thesis. Two sources of spurious fluctuations [125] pertaining to diffuse interface IB methods are attributed to spatial discontinuity in pressure across the immersed surface in newly born fluid nodes and the temporal discontinuity in velocity of dead fluid nodes. The spurious oscillations are comparatively more significant in pressure transients than the viscous forces and hence may be quantified using the 2δ -discontinuity in the temporal history of the pressure drag coefficients as expressed in Eq. (3.6). In the present study, the grid resolutions are varied as $\Delta x/d = 1/16, 1/32, 1/64$ and $1/128$ while maintaining constant relaxation factor $\tau_f = 0.65$.

Figure 5.10a depicts the root-mean-square values of 2δ -discontinuity in pressure

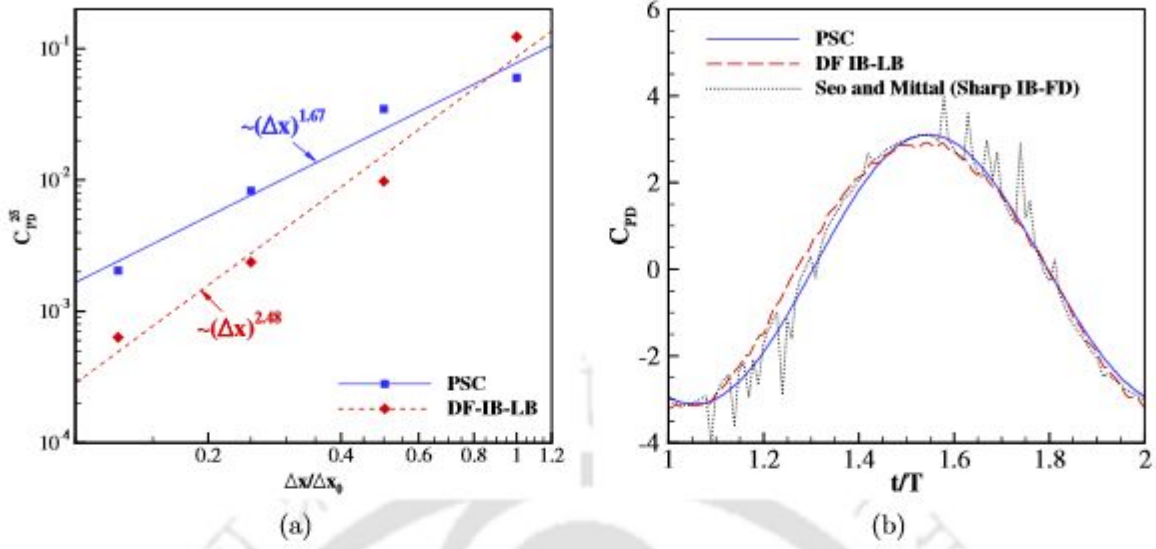


Figure 5.10: (a) $C_{PD}^{2\delta}$ discontinuity as a function of grid resolution using PSC and DF-IB-LB methods. (b) Comparison of spurious fluctuation in pressure drag coefficient (C_{PD}) using PSC, DF-IB-LB and sharp IB-FD method proposed by Seo and Mittal [95].

drag coefficient, where Δx_0 represents the coarsest grid resolution ($d/16$). The best-fit power-law curve through the discrete values reveals that $C_{PD}^{2\delta}$ decays approximately at a rate of 2.48 using the DF-IB-LB approach, which is higher than near-quadratic decay reported by Seo and Mittal [95] for sharp-interface immersed boundary-finite volume (IB-FV) method and approximately a linear decay ($C_{PD}^{2\delta} \sim (\Delta x)^{1.31}$) using a volume-of-body IB-FV solver [81]. However, the decay of the same at a rate of 1.67 using the PSC approach is comparable to that obtained by Seo and Mittal [95] and De [81]. In addition to it, the comparison of the temporal history of pressure drag coefficient (C_{PD}) (Fig. 5.10b) using PSC and DF-IB-LB with sharp-interface IB-FV [95] confirms the efficacy of both DF-IB-LB and PSC towards smooth estimation of aerodynamic forces in moving boundary problems. It can also be observed that the PSC method obtained smoother C_{PD} signal as compared to the DF-IB-LB approach. Hence, the present investigation enlightened that PSC methodology can diminish SFOs with grid refinement comparable to the conventional IB-FV and DF-IB-LB solvers.

5.5 Galilean invariance study

The study of Galilean invariance in the context of comparative analysis of the DF-IB-LB and PSC approaches is important given that conventional approaches with momentum-exchange method [88] in LBM at the fluid-solid interface are known to exhibit non-Galilean invariance behavior. In addition, there have been algorithmic

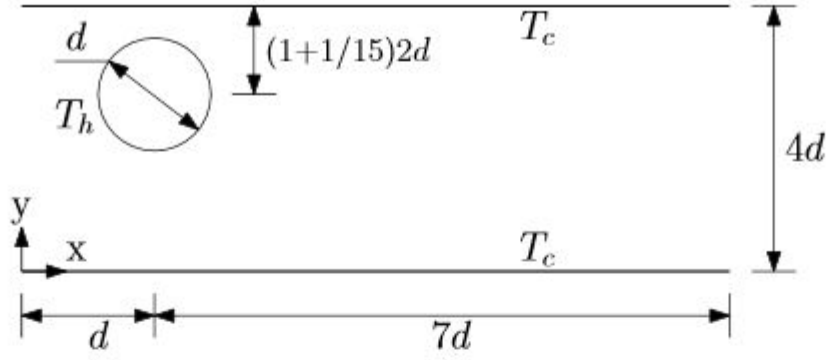


Figure 5.11: Schematic representation of the computational domain of a cylinder in a Couette flow. This figure is identical to Fig. 4.7. It is put here to enhance the readability of the chapter.

improvements for the momentum-exchange method [126, 127], but no such studies were found forthcoming in the DF-IB-LB framework. The Galilean invariance study ensures that the method will yield an identical flow field irrespective of using a stationary or moving reference frame. Or in other words, the underlying computational framework is independent of the choice of reference frame for a moving body problem. Towards this objective, the test case of the transient Couette flow past a moving cylinder is considered which is inspired by the work of Lallemand and Luo [34] and formerly presented in Section 4.2 of this thesis.

A circular cylinder with diameter d and higher temperature (T_h) is eccentrically placed in a channel of domain size $8d \times 4d$ as shown in Fig. 5.11. Two inertial frames are considered in this study, with the first being a stationary (rest frame) where the initial flow field (U_0) and the moving cylinder (U_c) velocities in x -direction are prescribed as 0.02 m/s. The upper and bottom walls (U_w) of the channel were moving with a constant velocity of 0.1 m/s opposite to each other in x -direction and maintained at lower temperature (T_c). At LB-level, no-slip boundary conditions on channel walls are implemented using the non-equilibrium bounce back method proposed by Zou and He [11] while in x -direction, periodic boundary conditions are applied. The temperature boundary conditions at domain boundaries are implemented following the method proposed by Liu et al. [86]. The second scenario is the moving reference frame with a constant reference velocity ($U_{ref} = -0.02$ m/s in x -direction. The cylinder thus becomes static with $U_c + U_{ref} = 0.0$ m/s, and the initial condition of the flow field becomes quiescent $U_0 + U_{ref} = 0.0$ m/s as well. The upper wall gains a velocity of $U_w + U_{ref} = 0.08$ m/s whilst the velocity of the bottom wall becomes $U_w + U_{ref} = -0.12$ m/s. The simulation parameters for either scenarios are set as $Re = d^2 \kappa / \nu_f = 11.36$, $\tau_f = 0.714$ and physical diameter of the cylinder as $d = 0.05$ m. The shear rate of the flow is chosen as $\kappa = 2U_w/4d$ where ν_f represents the kinematic viscosity of the fluid.

The time variation of the aerodynamic force coefficients depicted in Fig. 5.12

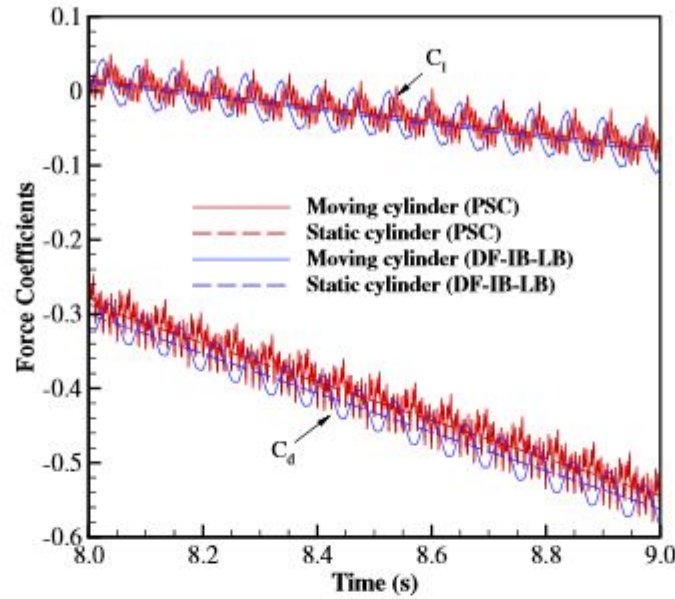


Figure 5.12: Time variation of aerodynamic force coefficients of a cylinder in a Couette flow in moving and static reference frames at $Re = 11.36$ and $\tau_f = 0.714$ using PSC and DF-IB-LB methods.

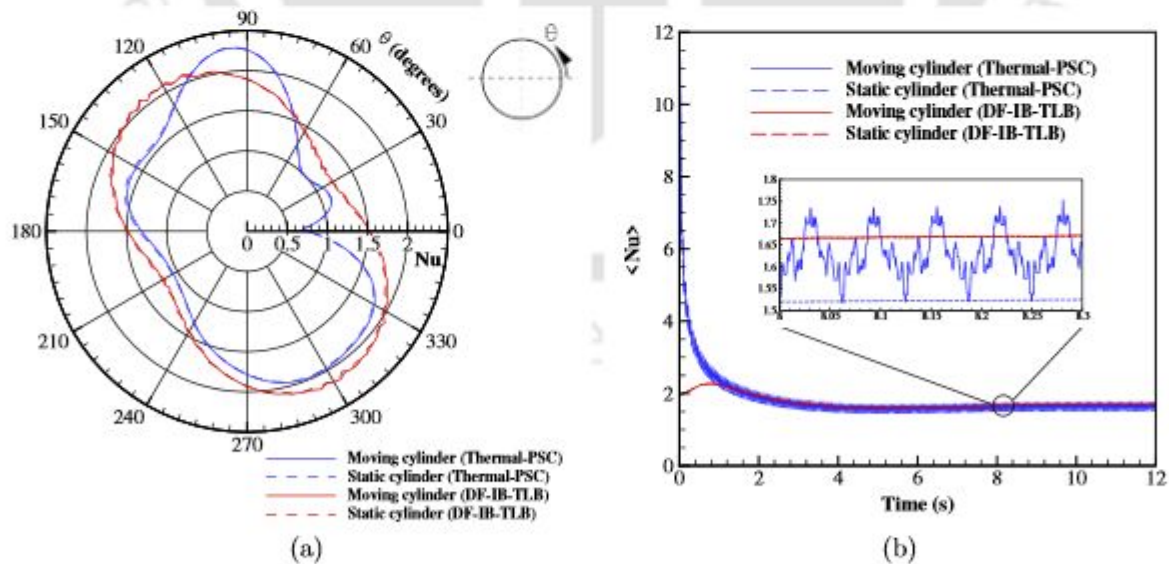


Figure 5.13: Comparison of (a) local Nusselt number distribution as a function θ at time ($t = 10.0s$) and (b) average Nusselt number as a function of time using PSC and DF-IB-LB methods.

suggests that oscillatory signals in the moving cylinder cases follow it's mean close to the signal obtained in the stationary cylinder cases. It can be observed that the PSC signals exhibit more fluctuations than the DF-IB-LB data. Nevertheless, both approaches follow Galilean invariance in incompressible flows involving complex structures. Furthermore, the local Nusselt distribution as a function of θ and the average Nusselt number as a function of time illustrated in Fig. 5.13 signifies that PSC and DF-IB-LB methods are Galilean invariant in thermo-fluidic applications.

5.6 Summary

The present chapter demonstrates a comparative analysis of the PSC and the DF-IB-LB approaches targeting four facets of numerical appraisal, viz., accuracy, discrete conservation of properties, spurious force oscillations in moving boundary problems, and Galilean invariance in thermo-fluidic applications. The major inferences from the investigation are summarized as follows

- The accuracy study reveals that the velocity and temperature error norms decay linearly, while the pressure error exhibits a second-order convergence with grid refinement.
- The τ_f sensitivity analysis infers that the velocity and temperature errors using PSC increases with an increase in τ_f , while they decrease until $\tau_f = 1.5$ and $\tau_f = 1.6$, respectively, beyond which they exhibit an increasing trend using the DF-IB-LB approach. However, the pressure error norms exhibit a monotonic increase in error with the increasing τ_f and carry the identical magnitude of errors for both approaches.
- The study on discrete conservation of properties reveals that the PSC approach possesses a lower magnitude of local maximum divergence than the DF-IB-LB approach. Furthermore, the mass flux error and the maximum density fluctuations decay with grid refinement in PSC and DF-IB-LB approaches. On the contrary, the maximum density fluctuations increase with an increase in τ_f in both approaches.
- The spurious force oscillations in moving boundary problems decay at a rate of 2.48 with respect to the grid refinement using the DF-IB-LB approach, while the same exhibits the decay at a rate of 1.67 using the PSC method. Nevertheless,

the PSC method obtains a smoother pressure drag signal in comparison to the DF-IB-LB approach.

- The study of hydrodynamic and thermal characteristics using PSC and DF-IB-LB methods in moving and stationary reference frames reveal that both methods are Galilean invariant in thermo-fluidic applications.

In light of the above conclusions, it can be inferred that the PSC approach predicts accurate thermo-fluidic characteristics in complex moving boundary problems, which is comparable to the conventional DF-IB-LB method.



CHAPTER 6

PARTIALLY SATURATED CELLS APPROACH FOR CONJUGATE HEAT TRANSFER PROBLEMS

“If anyone thinks that all of our developments took place in a direct fashion with no glitches along the way, I have to assure you that lots of false starts and turns occurred in virtually every project that we undertook”

- Francis H. Harlow, *J. Comp. Phys.*, 195 (2004) 414-433

This chapter proposes a unified governing equation for the fluid and solid media undergoing the conjugate heat transfer process. The proposed algorithm is based on the partially saturated computational cells method that so far has proven to be an accurate and efficient methodology for treating complex boundaries which are not aligned with the underlying Cartesian grid. The state-of-the-art literature survey for conjugate heat transfer (CHT) problems using the lattice Boltzmann method highlights that most of the popular algorithms in this topic either reconstruct the unknown energy distribution function or add an additional source term to satisfy the interfacial boundary conditions. Very limited work utilizes the immersed boundary method for CHT problems, let alone the PSC approach. The chapter discusses the development of the proposed algorithm and validates the solver with respect to non-trivial benchmark problems encompassing free, forced, and mixed convection phenomena. Furthermore, the inferences from these test cases motivates the author to present a novel strategy for the implementation of adiabatic boundary conditions using the PSC approach, which hitherto has not been discussed in the open literature.

The conjugate heat transfer phenomena arise from the coupled thermal interactions between the solid and fluid media having a common solid-fluid interface. The

utility of this phenomenon can be found in a large variety of industrial applications such as nuclear reactors, blade cooling in jet engines, micro-devices, electronic cooling, chemical processes, etc. The interface boundary conditions applicable for CHT problems comprise two crucial physical requirements: (i) continuity of temperature and (ii) continuity of heat flux. Let us consider a solid-fluid interface across which the CHT phenomena may occur, as depicted in Fig. 6.1. The conjugate condition at the interface can then be mathematically expressed as

$$T|_f^I = T|_s^I \quad (6.1)$$

$$\eta \cdot (k_f \nabla T) \Big|_f^I = \eta \cdot (k_s \nabla T) \Big|_s^I \quad (6.2)$$

Here η , I , f and s represent the normal vector to the surface, interface, fluid, and solid, respectively. Computational solution techniques used in literature to solve these interface conditions in CHT problems can be broadly classified as partitioned and monolithic approaches. The partitioned approach enforces the interface boundary conditions of continuity of heat flux and temperature explicitly on the solid-fluid interface while separately solving the energy equation in the solid and fluid domain. It further requires extrapolation of temperature and heat fluxes at the interface. Additionally, the implementation of Neumann boundary condition on curved surface using conventional thermal bounce-back like schemes [128] involve special interpolation and extrapolation techniques [129] owing to the determination of more than one unknown distribution function at the boundary. Hence the conjugate heat transfer problems involving complex interface geometry necessitate considerable computational efforts and

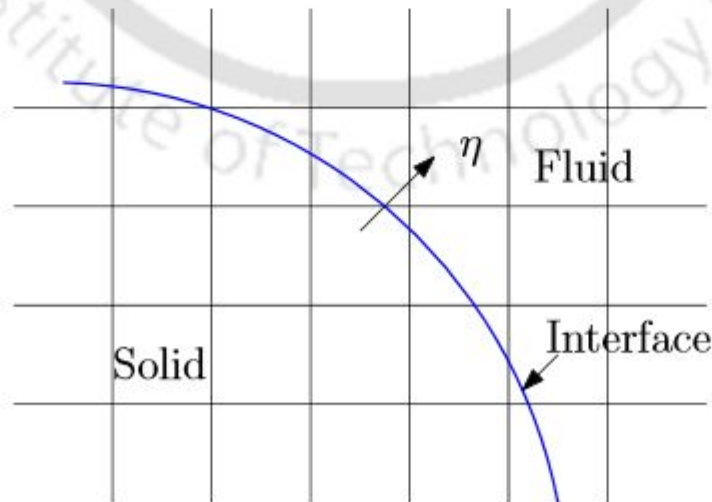


Figure 6.1: Schematic showing a solid-fluid interface during conjugate heat transfer problem.

complex algorithms. In contrast to the partitioned approach, the monolithic approach offers a single governing equation for energy over the entire computational domain, irrespective of the solid and fluid media present. Compared to the monolithic approach, the partitioned approach, in conjunction with the immersed boundary method, requires additional bookkeeping for identifying fluid and solid immersed cells to couple temperature across the solid-fluid domains. In the subsequent paragraphs, a comprehensive survey of the numerical methodologies is presented which is developed so far to simulate CHT problems using the LB method.

Wang et al. [130] proposed an algorithm for conjugate heat transfer that includes a generalized heat source term in the TLBM capable of including the viscous dissipation and pressure compression effects. The temperature and heat flux continuities at the solid-fluid interface are insured by a "half-lattice division" scheme presented by them. This method utilizes a half-way bounce-back model for the flow evolution equation at the interface, while for the heat transfer evolution equation, local solid or fluid properties are obtained using the interfacial constraints. The proposed algorithm is validated for pure heat conduction and flow through a heated thick-wall microchannel against classical CFD solvers, where straight interfaces are placed at the center of the lattice links. The half-lattice division approach proposed by Wang et al. [130] and Chen and Han [131] obtains thermal relaxation time from the respective local properties of the solid or fluid nodes; however, no interface nodes were considered for such calculations. The algorithm followed by Wang et al. [130], also known as the pseudo-density approach, replaces each node's density by its heat capacitance (ρc_p). Whereas Chen and Han [131] suggested that solid and fluid heat capacitance could be equated at the interface to apply the interface boundary conditions.

In contrast to the half-lattice division approach, Seddiq et al. [132] proposed a scheme for interface treatments by considering lattice nodes exactly on the fluid-solid boundary. The non-tangential energy distributions of these interfacial nodes were obtained using an interpolation function that utilizes the energy distributions of neighboring nodes and respective relaxation times of solid-fluid nodes as weighting factors. The tangential energy distribution functions were evaluated by supposing the difference of these distribution functions is proportional to their difference of post-streaming values. Finally, the interface temperature is obtained as a summation of these interfacial distribution functions. In another approach, Meng et al. [133] utilized the equilibrium of counter-slip internal energy [134] with the thermal boundary-condition at the solid-fluid interface for simulating CHT in high-frequency oscillating flows. The method consists of two separate models of internal energy distribution function for

the solid and the fluid medium. The unknown distribution functions at the solid-fluid interface are obtained using the counter-slip internal energy for each unknown, which is determined using the temperature and heat flux continuity constraints at the interface. Unlike the half-lattice division approach, this scheme requires the interface to be located precisely on the lattice nodes.

So far, the LBM schemes for CHT problems have been limited to straight interface geometries. Li et al. [135] proposed a generalized method to treat curved interfaces, eliminating the existing techniques of coupling interfacial fluxes along the discrete velocity direction. Guo et al. [136] extended the work of Li et al. [135] that treats the interfacial jump conditions intrinsically eliminating the need for iterative computations as compared to that followed in conventional FDM and FVM solvers. Apart from that, the scheme relies on the interface topology, and needless to say, the complicated formulation of associated coefficients needs to be tuned accordingly.

The algorithmic limitations of the node or link-based LB schemes can effectively be alleviated using coupled immersed boundary-lattice Boltzmann method. One such exposition pertaining to conjugate heat transfer problems was highlighted in the work of Hu et al. [137]. They utilized the 'pseudo-solid-specific-heat' technique to implement heat flux continuity at the solid-fluid interface which suggests that the ratio of heat capacitance of solid to that of fluid under steady-state conditions equals one. Unlike the half-lattice-division technique, the conjugate conditions at the interface are sought by invoking a double distribution model of TLBM with zero value for the source term.

When considering different heat capacitance for solid and fluid media, the pseudo-specific-heat approach fundamentally fails to recover the standard energy equation from the conventional TLBM approaches. To address this issue, Lu et al. [138] proposed a 'virtual-heat-capacity-correction' based LB algorithm for CHT problems. Initially, it assumes equal heat capacitance of solid and fluid media to ensure the continuity of heat flux at the interface and then rectifies the temperature and distribution functions by considering unequal heat capacitance at the end of each time step. In addition to the steady state cases, the method can be successfully implemented to the transient conjugate problems but limits its applicability for $(\rho c_p)_s/(\rho c_p)_f \geq 1$ conditions and stationary cases only. In another approach proposed by Lu et al. [139], a corrected streaming step is devised based on the difference method, which ensures that the adjacent nodes to the interface obtain distribution functions from the interface nodes. The interfacial distribution functions are evaluated by coupling the continuity

of temperature and heat flux using a non-equilibrium extrapolation scheme. Although the method can reliably predict steady and transient problems but limits its interface topology to staircase-like approximation.

Mu et al. [140] proposed a general interface formulation for conjugate heat and mass transfer problems which considers either the continuity or discontinuity of interfacial conditions. The unknown distribution functions at the interface are obtained utilizing the existing post-collision distribution functions along with the interfacial jump conditions. Hosseini et al. [141] proposed an energy evolution equation that deals with variable specific heat capacity and recovers the conservative form of the total sensible energy transport equation. The modified equilibrium distribution function proposed by them eliminates the inconsistencies of heat flux at the solid-fluid interface while considering unequal heat capacities of solid and fluid media. Kumar and Natarajan [87] proposed a diffuse-interface monolithic immersed boundary conjugate heat transfer algorithm that utilizes unified governing equations for momentum and energy across the entire computational domain. The solver is based on the finite-volume method and shows that it can predict the interfacial heat transfer characteristics in accordance with the existing literature for natural and forced convection problems. The local Nusselt number distribution over curved surfaces shows significant spurious oscillation over curved surfaces but exhibits a good match in the prediction of averaged quantities.

The above comprehensive survey of literature for CHT problems using LBM suggests that the interface treatment strategies can be broadly classified into two categories: (1) reconstruction of unknown populations depending upon the interface geometries [132, 133, 142] and (2) addition of source terms specifically to the nodes near the interface instead of correcting the unknown populations [143, 144]. Despite having promising features in the IB-LB method to account for the accurate implementation of the boundary conditions on complex structures, very limited work was found for the simulation of CHT problems, let alone no literature reports the utilization of PSC methodology for such problems as per the author's knowledge. The primary reason behind it can be attributed to the complex implementation of the CHT interfacial boundary conditions. The present thesis proposes a unified thermal evolution equation for simulating the conjugate heat transfer problems using the partially saturated computational cells method. The PSC governing equation for CHT problems can be mathematically expressed as

$$g_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - g_i(\mathbf{x}, t) = (1 - \Phi_B) \Psi_i^{BGK} + \Phi_B \Psi_i^{B,CHT} \quad (6.3)$$

$$\Psi_i^{B,CHT} = \frac{\Delta t}{\tau_{g,s}} [g_i^{eq}(\rho, \mathbf{U}_p, T) - g_i(\mathbf{x}, t)] \quad (6.4)$$

where, the dimensionless relaxation time ($\tau_{g,s}$) for solid cells can be related to their thermal diffusivity as

$$\chi_s = 2(\tau_{g,s} - 0.5)c_s^2\Delta t \quad (6.5)$$

Here Φ_B represents the volume fraction of the immersed solid and signifies the similar meaning in the thesis described in the section 2.2.1. In order to account for the interfacial boundary conditions, the proposed methodology neither modifies the energy distribution function nor adds any additional source term to the governing equations, unlike the LB schemes mentioned above schemes. Instead, the BGK collision operator explicitly takes care of the boundary conditions because of its simplicity and ease of implementation. It must be mentioned here that under steady-state conditions, the thermal conductivities of the medium play a crucial role in obtaining the temperature distributions in the conjugate heat transfer problems. Hence the applicability of the heat capacitance (ρc_p) becomes irrelevant in such conditions, and one can represent the ratio of heat capacitance of solid to that of the fluid medium as the ratio of their respective thermal conductivities ($\chi_s/\chi_f \sim k_s/k_f$) [131]. A brief strategy to obtain the relevant LB parameters in CHT problems using the proposed methodology is illustrated in the Algorithm 4. The subsequent sections of this chapter will now present the efficacy and robustness of the present PSC solver to simulate CHT phenomena involving straight and curved boundaries for a wide range of non-trivial benchmark problems.

Algorithm 4: Computational strategy for implementation of partially saturated computational cells method in conjugate heat transfer simulations.

Grid generation;
 Set $\tau_f, Pr, k_s/k_f$, characteristic dimensions (say H) and governing non-dimensional numbers like Re, Gr, Ri etc.;
 Obtain ν_f following the Eq. 2.5;
 Evaluate $g\beta = Gr\nu_f^2/\Delta TH^3$ (Applicable for free and mixed convection problems);
 Evaluate the thermal diffusivity of the fluid medium as $\chi_f = \nu_f/Pr$;
 Find $\tau_{g,f} = \frac{\chi_f}{2c_s^2\Delta t} + 0.5$;
 Obtain the thermal diffusivity of solid as $\chi_s = \frac{k_s}{k_f}\chi_f$;
 Find $\tau_{g,s} = \frac{\chi_s}{2c_s^2\Delta t} + 0.5$;
 Evaluate characteristics velocity (if applicable);
 Initialization;
for each time step t do
 Obtain solid volume fraction Φ_B at each cell;
 Obtain discrete forcing term using 2.14 (if applicable);
 Apply PSC governing equations via collision and streaming steps alongwith the evaluation of solid collision operator for each cell [Eq. (2.18b) or Eq. (2.18a)];
 Apply hydrodynamic boundary condition at domain boundaries following Zou and He [11];
 Evaluate macroscopic variables using Eqns. (2.4a) and (2.4b);
 Apply PSC evolution equation for CHT using Eq. 6.3, via collision and streaming operations;
 Apply thermal boundary conditions at domain boundaries following Liu et al. [86];
 Evaluate macroscopic temperature (T) using Eq. 2.11 ;
 Modify fluid velocity using a corrector step as 2.15.
end

6.1 Conjugate natural convection in a cavity

The natural convection in a cavity having a thick wall is chosen as the first problem to validate the CHT solver. The square cavity comprises size H where a thick wall of width $0.2H$ is immersed into it, resulting in a computational domain of size $1.2H \times H$. The grey and white shade in Fig. 6.2 depicts solid and fluid zone, respectively. Though the solid-fluid interface is parallel to the vertical boundaries but is located such that it does not align with the grid lines. The intention for selecting such a configuration is to adjudge the efficacy of the PSC solver subjected to non-binary solid volume fractions. Thus the interface cells in the present problem possess solid volume fraction value as $\Phi_B = 0.5$. The boundary conditions for the temperature of the problem can be expressed as $T(0, y) = T_c$, $T(1.2H, y) = T_h$ and $T'_y(x, 0) = T'_y(x, H) = 0$, where T'_y signifies $\partial T / \partial y$. The simulations are conducted for three different thermal conductivity ratios and Grashof number viz., $k_s/k_f = 1, 5, 10$ and $Gr = g\beta\Delta TH^3/\nu_f^3 = 10^5, 10^6, 10^7$. The computational domain comprises 480×400 lattice nodes, while the Prandtl number and relaxation time of the Boussinesq fluid across all the simulations is set as $Pr = 0.7$ and $\tau_f = 0.6$, respectively. Fig. 6.3a reveals that the non-dimensional temperature profiles ($\Theta = (T - T_c)/(T_h - T_c)$) at the solid-fluid interface for different thermal conductivity ratios at $Gr = 10^7$ show an excellent agreement with that obtained by Pan et al. [145]. It further indicates that with the increase in (k_s/k_f) , the thermal conduction through the solid wall increases and results in an increase in the temperature. Furthermore, the increase in temperature along the vertical direction across all cases of thermal conductivity ratios can be attributed to the downward and upward movement of fluid along the cold and hot walls of the cavity, respectively. The variation of local Nusselt number along the vertical direction in Fig. 6.3b reveals that the thermal

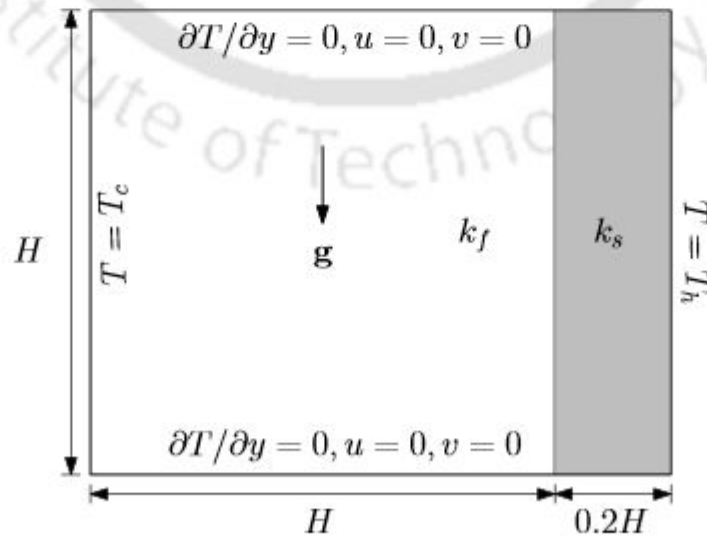


Figure 6.2: Schematic showing the natural convection in a cavity.

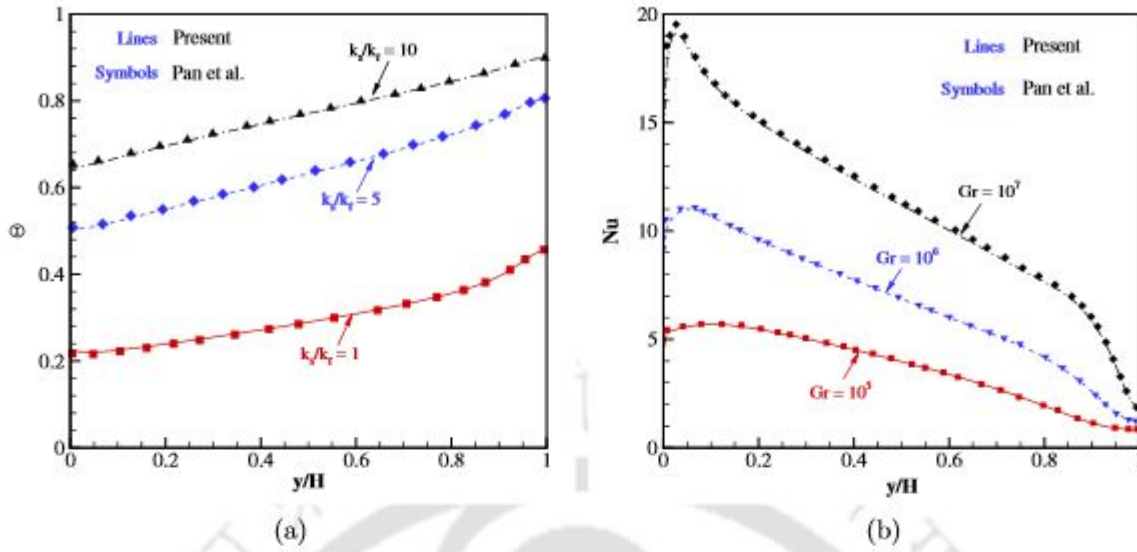


Figure 6.3: Comparison of (a) temperature for $Gr = 10^7$ and (b) local Nusselt number for $k_s/k_f = 10$ at the solid-fluid interface with respect to data reported by Pan et al. [145].

Table 6.1: Comparison of the average Nusselt number for different values of Grashof numbers and thermal conductivity ratios at solid-fluid interface with the data reported by Pan et al. [145]

$\frac{k_s}{k_f}$	$Gr = 10^5$		$Gr = 10^6$		$Gr = 10^7$	
	Present	Pan et al. [145]	Present	Pan et al. [145]	Present	Pan et al. [145]
1	2.07	2.08	2.84	2.85	3.47	3.51
5	3.39	3.41	5.82	5.85	8.91	9.01
10	3.69	3.70	6.73	6.76	11.19	11.30

convection strengthens with an increase in Grashof number at a fixed $k_s/k_f = 10$. The decrease in the Nusselt number with an increase in y/H value can be attributed to the increase in boundary layer thickness along the vertical direction at location $x/H = 1$. This can further be visualized in isotherm contours in Fig. 6.4. An excellent agreement of local Nusselt number at the solid-fluid interface with respect to that obtained by Pan et al. [145] depicted in Fig. 6.3b suggests that the present PSC solver is efficient enough to capture local thermal characteristics along straight interfaces in CHT problems. Table 6.1 further asserts that the average Nusselt number for different values of Grashof number and thermal conductivity ratios at the solid-fluid interface is in good agreement with that reported by Pan et al. [145] and within 1.2% relative error.

Further an exercise is performed to evaluate the temperature gradient utilizing the fluid and solid side lattice nodes separately. Let us consider the location of the solid-fluid interface is represented as I . The temperature gradient at the adjacent fluid location, i.e., at $(I - 1)$ lattice node, be represented as $\langle \partial T / \partial x|_{I-} \rangle$. Similarly

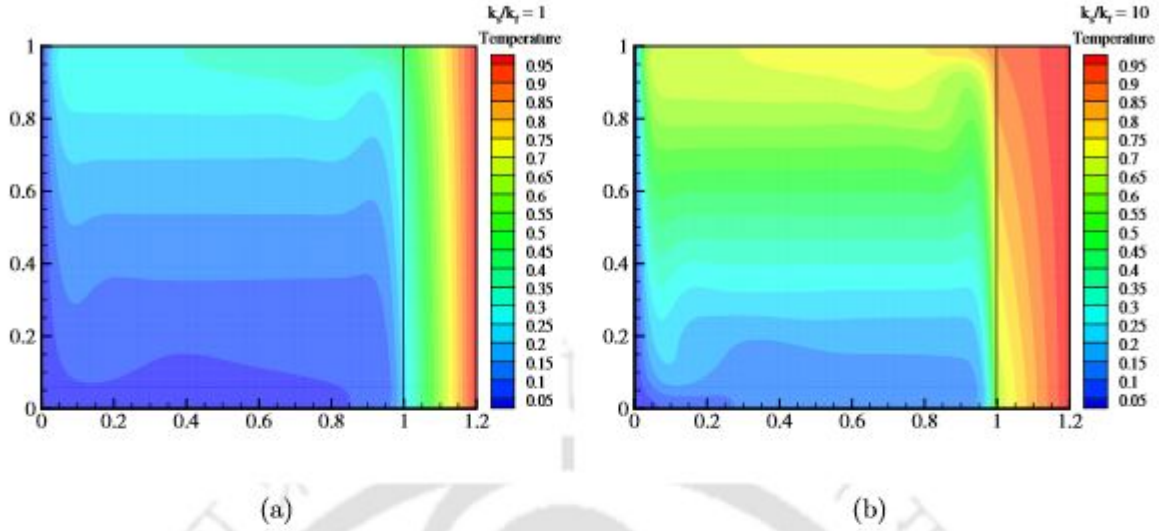


Figure 6.4: Isotherms at thermal conductivity ratio (a) $k_s/k_f = 1$ and (b) $k_s/k_f = 10$ for conjugate natural convection in a cavity.

Table 6.2: Temperature gradient utilizing the fluid and solid side nodes of the interface.

k_s/k_f	$\langle \partial T / \partial x _{I-} \rangle$ Fluid side	$\langle \partial T / \partial x _{I+} \rangle$ Solid side	$\langle \partial T / \partial x _{I-} \rangle / \langle \partial T / \partial x _{I+} \rangle$
1	0.00868	0.00874	0.993
5	0.02228	0.00451	4.940
10	0.02797	0.00285	9.814

the solid side temperature gradient be represented as $\langle \partial T / \partial x |_{I+} \rangle$. These gradients are evaluated using a second-order backward or forward difference scheme, which utilizes the temperature of the fluid and solid nodes, respectively. The ratio of the fluid side to the solid side temperature gradient for all cases of thermal conductivity ratios are presented in Table 6.2. It must be noted that the ratio of temperature gradient $\langle \partial T / \partial x |_{I-} \rangle / \langle \partial T / \partial x |_{I+} \rangle$ corresponds to the ratio of calculated thermal conductivity ratio.

$$\frac{\langle \partial T / \partial x |_{I-} \rangle}{\langle \partial T / \partial x |_{I+} \rangle} \sim \frac{\langle \partial T / \partial x |_f \rangle}{\langle \partial T / \partial x |_s \rangle} \approx \left. \frac{k_s}{k_f} \right|_{\text{calculated}} \quad (6.6)$$

The above exercise is carried out at identical grid resolution for all cases considered here. It can be observed that the calculated thermal conductivity ratio is within 2% relative error with respect to the input thermal conductivity ratio. The small deviation at large thermal conductivity ratio can be minimized with finer grid resolution. This particular analysis and the data shown in Table 6.2 guarantees that the present PSC solver ensures the continuity of heat flux at the straight solid-fluid interface. The subsequent sections will present the efficacy of the PSC solver to simulate conjugate

heat transfer across curved boundaries.

6.2 Forced convective conjugate heat transfer: Flow past a heated non-homogeneous circular cylinder

The present section deals with validating the PSC solver for the conjugate heat transfer process across curved surfaces that are not aligned with the underlying Cartesian mesh. A forced convective phenomena past a heated non-homogeneous circular cylinder is considered for the study. A cold stream having temperature T_c flows over a concentric cylinder whose inner core is heated at temperature T_h . The diameter of the inner core is half of the outer cylinder's diameter (d). The cylinder is located at $(6d, 6d)$ in a computational domain of size $20d \times 12d$ whose boundary conditions are illustrated in Fig. 6.5. The present test case is performed for four different thermal conductivity ratios viz., $k_s/k_f = 0.5, 1, 4, 20$ at $Re = U_d/\nu_f = 40$ and $Pr = 0.72$. The LB level simulation parameter comprises 60 lattice nodes across the outer diameter of the cylinder while the relaxation time is set as $\tau_f = 0.6$ for all test cases in the present section. A comparative plot in Fig. 6.6 comprises of the non-dimensional temperature ($\Theta = T - T_c / T_h - T_c$) distribution over the outer cylinder's surface with respect to that obtained by Pareschi et al. [142] ensures the validity of the PSC solver. The increase in temperature with an increase in thermal conductivity ratio signifies the increase in heat conduction through the non-homogeneous zone of the cylinder. The temperature difference between the front and rear stagnation points increases with the decrease in

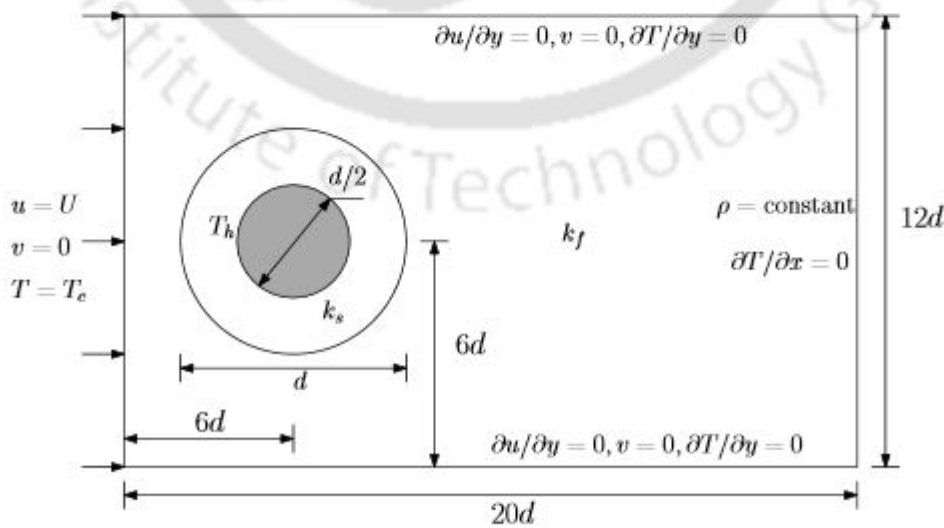


Figure 6.5: Schematic representation of forced convective heat transfer past a heated non-homogeneous circular cylinder (Figure not to scale).

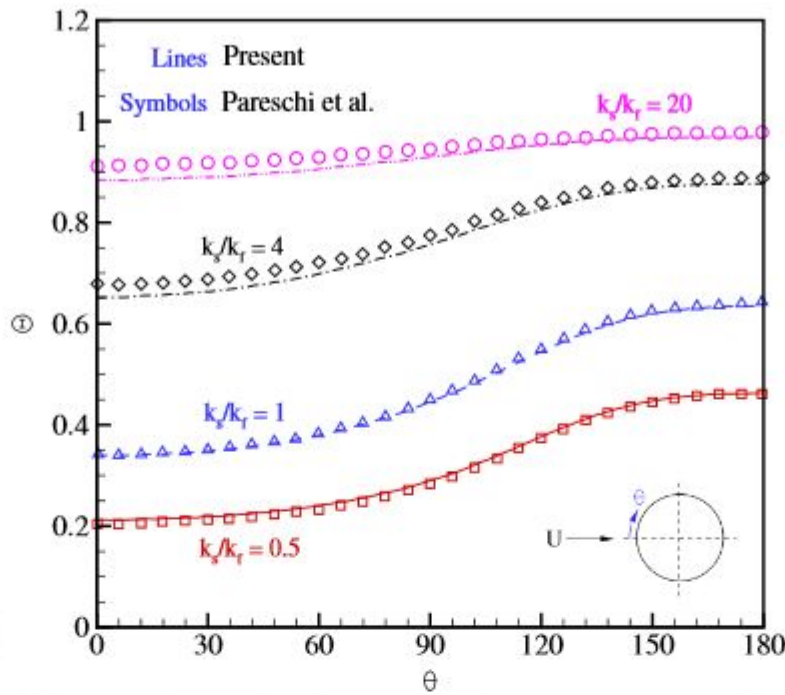


Figure 6.6: Comparison of temperature profile for different thermal conductivity ratios at the solid-fluid interface with respect to the data reported by Pareschi et al. [142] at $Re = 40$.

the thermal conductivity ratio. These can be further verified through the isotherms represented in Fig. 6.7. The local Nusselt distribution over the outer cylinder's surface is evaluated as per the Nu formulation depicted in the section 2.4.1. It must be mentioned that only fluid cells are utilized for the Dirac-delta interpolation of heat flux vectors from Eulerian nodes to the Lagrangian ones in the present PSC solver. The investigation reveals the oscillatory distribution of the Nusselt number over the curved surface for all cases of thermal conductivity ratio; however, only two such cases ($k_s/k_f = 0.5$ and 20) are shown for the brevity of the Fig. 6.8a. Such oscillatory behavior is in contrast to a smoother distribution obtained in the previous section despite the fact that both of these cases are not aligned with the underlying grid. It can be attributed to the fact that the solid-fluid interface in the preceding test case possesses a constant value of solid volume fraction, whereas it changes across the interface cells in the curved boundary problems. The solid volume fraction of the interface cell is a critical parameter in this class of diffuse-interface IB method as it influences the implementation of the boundary condition and the post-processing signals. Similar spurious signals in surface Nusselt number distribution were also reported in the diffuse interface IB-FV solver developed by Kumar and Natarajan [87]. Nevertheless, one can realize that the qualitative trend of the spurious signal follows close proximity to the data reported by Pareschi et al. [142]. To comprehend a smoother variation of

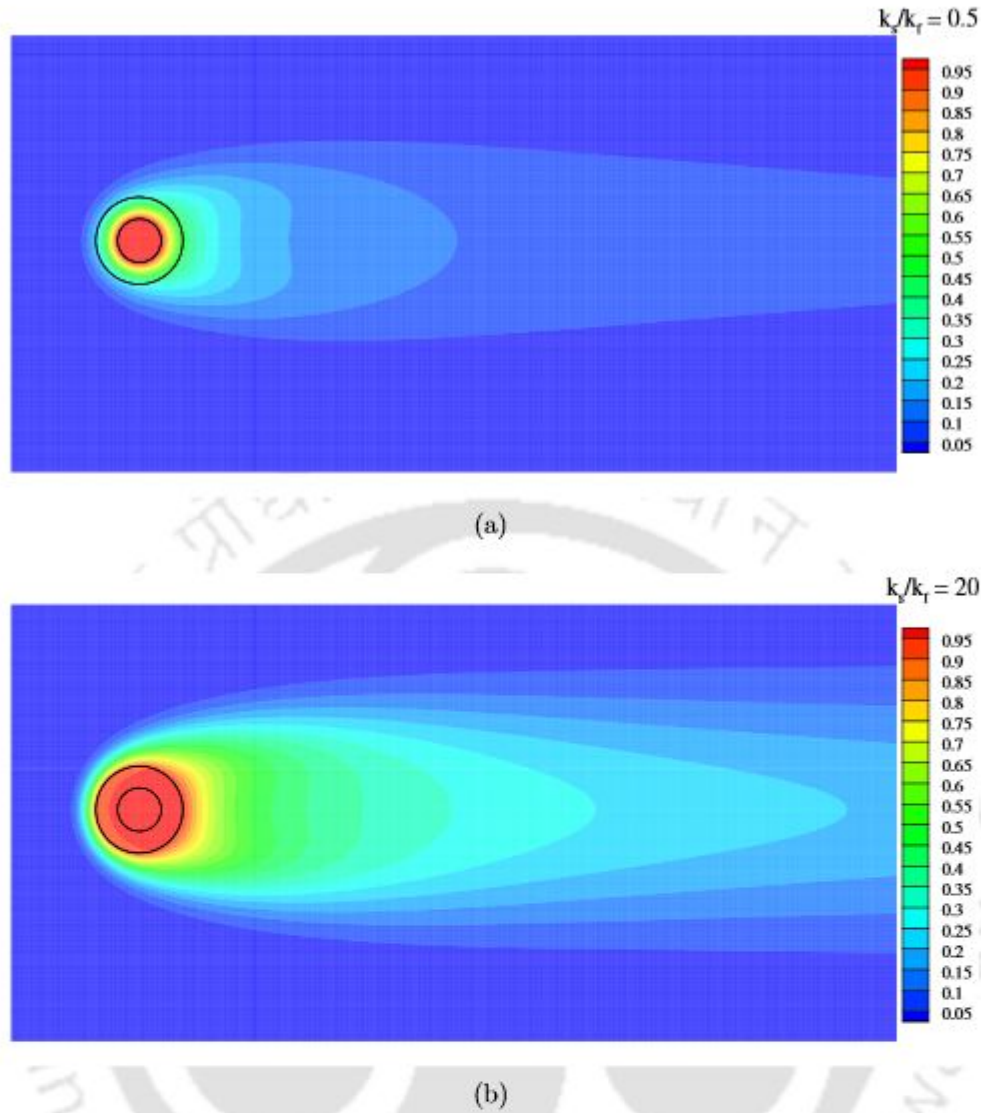


Figure 6.7: Isotherms of forced convective conjugate heat transfer for $Re = 40$ at thermal conductivity ratio (a) $k_s/k_f = 0.5$ and (b) $k_s/k_f = 20$

the surface Nusselt number, a low-pass filter is utilized to smoothen the data and the resulting signals are in good agreement with the Ref. [142] for all thermal conductivity ratios.

Furthermore, Fig. 6.8b portrays that with a decrease in k_s/k_f , the Nusselt number decreases and becomes flat along the cylinder's surface. Interestingly, it gives us a meaningful insight into the fact that a further decrease in the value of k_s/k_f might eventually decrease the temperature gradient towards zero. This limiting case would help devise an adiabatic condition at the cylinder's surface and will be deliberated in section 6.4.

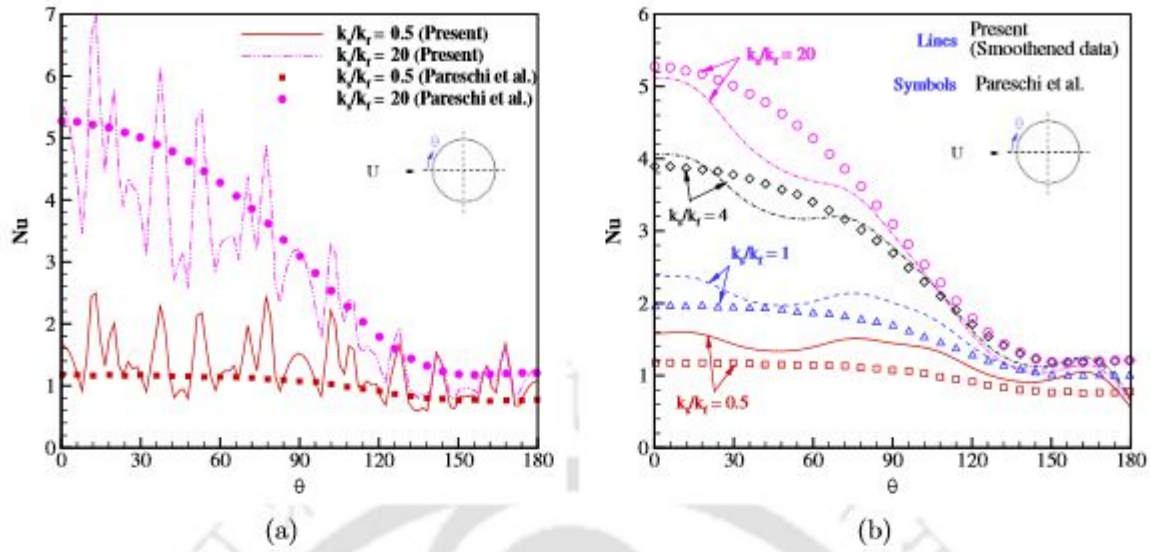


Figure 6.8: (a) Distribution of local Nusselt number along the fluid-solid interface and its comparison with Pareschi et al. [142] at $Re = 40$. (b) Smoothed distribution of the local interfacial Nusselt number using a low-pass filter for different thermal conductivity ratios at $Re = 40$.

6.3 Mixed convective conjugate heat transfer: Non-homogeneous circular cylinder in a lid driven cavity

In this section, a mixed convective conjugate heat transfer test case is carefully devised to validate the PSC solver. A non-homogeneous circular cylinder is immersed at the geometrical center of a square cavity of size H as illustrated in Fig. 6.9. The radii of the inner and outer cylinders are related to the cavity size as $r_i = 0.1H$ and $r_o = 0.2H$, respectively. The inner surface of the cylinder and the bottom wall of the cavity are prescribed higher temperature (T_h) than the temperature (T_c) of the top wall of the cavity to facilitate natural convection and conjugate heat transfer in the respective zones simultaneously. The left and right boundaries of the cavity are insulated. The top lid of the cavity is subjected to a uniform velocity (U). The present simulations are performed for three different thermal conductivity ratios, viz. $k_s/k_f = 0.1, 1, 10$ at Reynolds number $Re = UH/\nu_f = 100$. Three different types of convection, namely free, mixed, and forced convection, were investigated at Richardson number $Ri = Gr/Re^2 = 10, 1$ and 0.01 , respectively. The Boussinesq working fluid is considered as air having Prandtl number $Pr = 0.7$. All simulation cases comprise 250×250 lattice nodes in the cavity while the relaxation time (τ_f) is prescribed as 0.6 . Due to the lack of open literature for such a mixed convective CHT problem, the

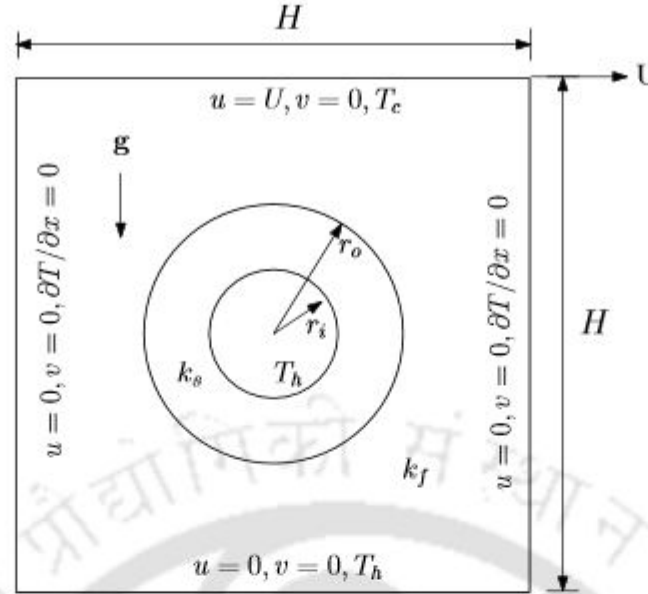


Figure 6.9: Schematic representation of mixed convective heat transfer through a heated non-homogeneous circular cylinder inside lid driven cavity.

present data are compared with a commercial finite volume solver, namely Ansys® Fluent. In Fluent simulations, the body-fitted grid around the cylinders is so created that its resolution is comparable to that prescribed in the present solver's setting. The setup comprises air as the working fluid with thermal conductivity as 0.0242 W/m-K. The thermal conductivity of the immersed solid is manually set in accordance to the selected thermal conductivity ratio (k_s/k_f) while the discretization scheme is followed identically to that mentioned in Section 4.3.5 of the thesis. Similar strategies are followed in Section 6.4 of the current chapter.

Fig. 6.10 represents a comparative plot of the distribution of local Nusselt number over the outer cylinder's surface with respect to that obtained using the Ansys® Fluent solver at $Ri = 10$ and $k_s/k_f = 10$. It is evident that although the Nu signal possesses severe spuriousness but maintains a good qualitative agreement with the Ansys® Fluent. Since such fluctuations are inevitable because of the diffuse-interface characteristics of the present solver, the Nu signals are presented for all the test cases by smoothening it through a low-pass filter in Figs. 6.11a, 6.11c and 6.11e. Furthermore, Figs. 6.11b, 6.11d and 6.11f illustrates the non-dimensionalized temperature ($\Theta = (T - T_c)/(T_h - T_c)$) profile along the solid-fluid interface for different cases of Ri and k_s/k_f . Additionally, the distribution of Nu over the heated bottom wall of the cavity for different cases of $Ri = 10$ and $k_s/k_f = 10$ is portrayed in Fig. 6.12. These figures assert that the present PSC solver can capture the local thermal characteristics around the curved solid-fluid interface and straight boundaries in mixed convective CHT problems and agrees well with that obtained using Ansys® Fluent.

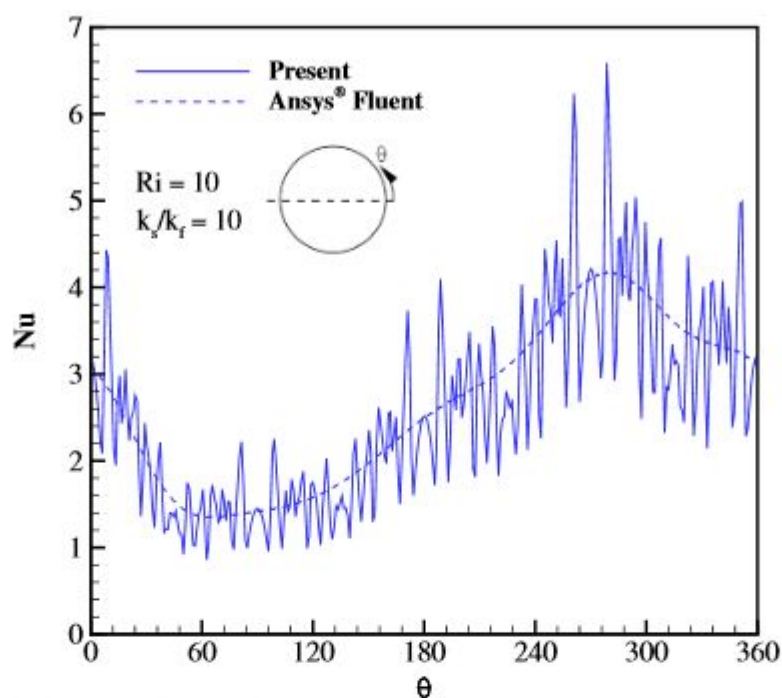


Figure 6.10: Comparison of local Nusselt number at solid-fluid interface with the Ansys® Fluent at $Ri = 10$ and $k_s/k_f = 10$.

Figs. 6.13, 6.14 and 6.15 illustrates the isotherm and streamline contours for $Ri = 0.01, 1$ and 10 respectively for different thermal conductivity ratios. At $Ri = 10$, greater homogenization of the temperature field is observed as compared to the lower Ri due to the significant buoyancy effect of the fluid in the former. The appearance of a recirculation eddy at the top right section of the cavity for $Ri = 0.01$ is evident due to the forced convective dominance of the flow field, which diminishes as the Ri increases. These figures also suggest that the temperature field of the non-homogeneous circular cylinder experiences the effect of the external flow field and is hence suggestive of the fact that the present solver satisfies the continuity of temperature and heat flux at the solid-fluid interface effectively.

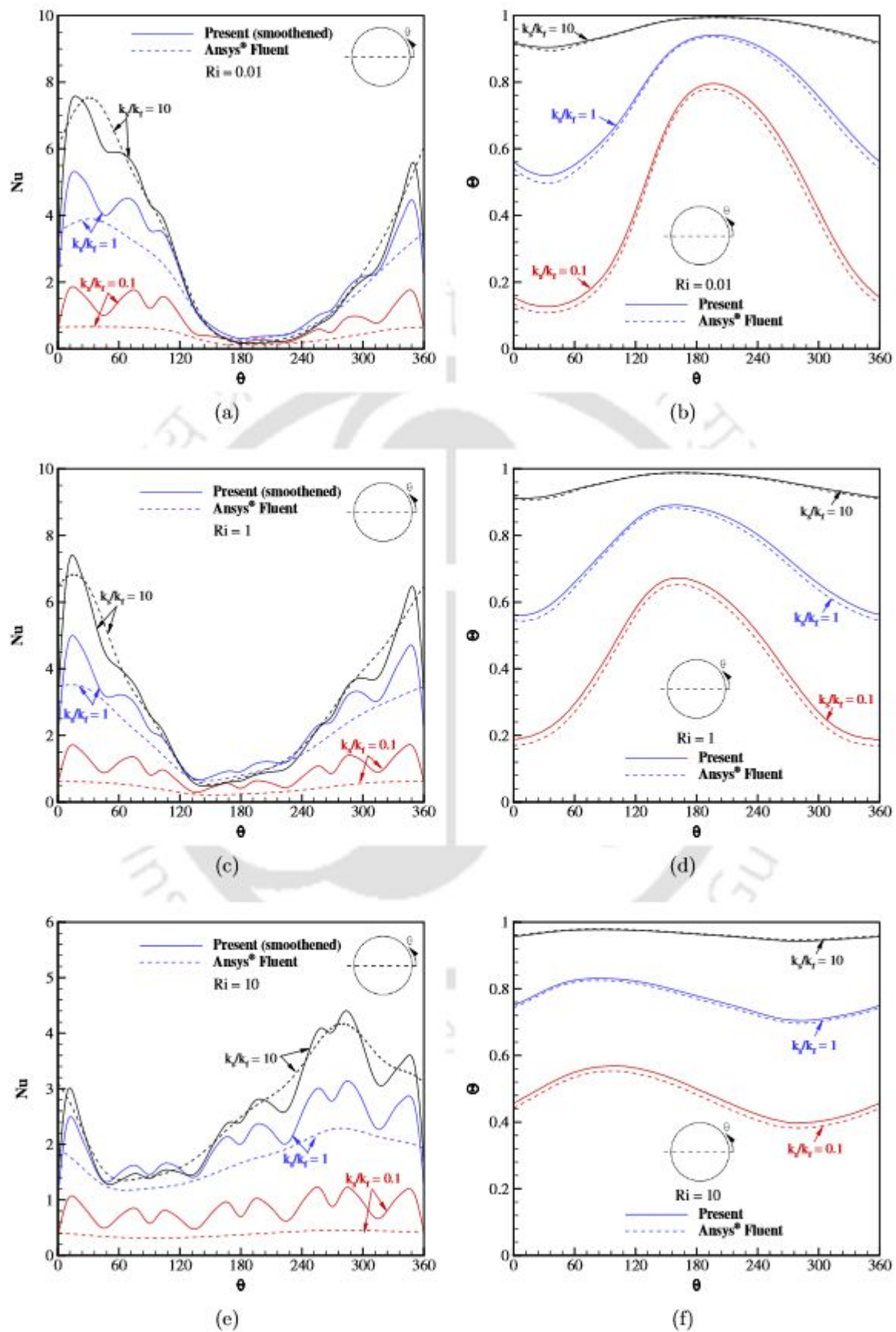


Figure 6.11: Distribution of local Nusselt number (smoothened) (Nu) and temperature profiles (Θ) at solid-fluid interface for different Richardson number and thermal conductivity ratios.

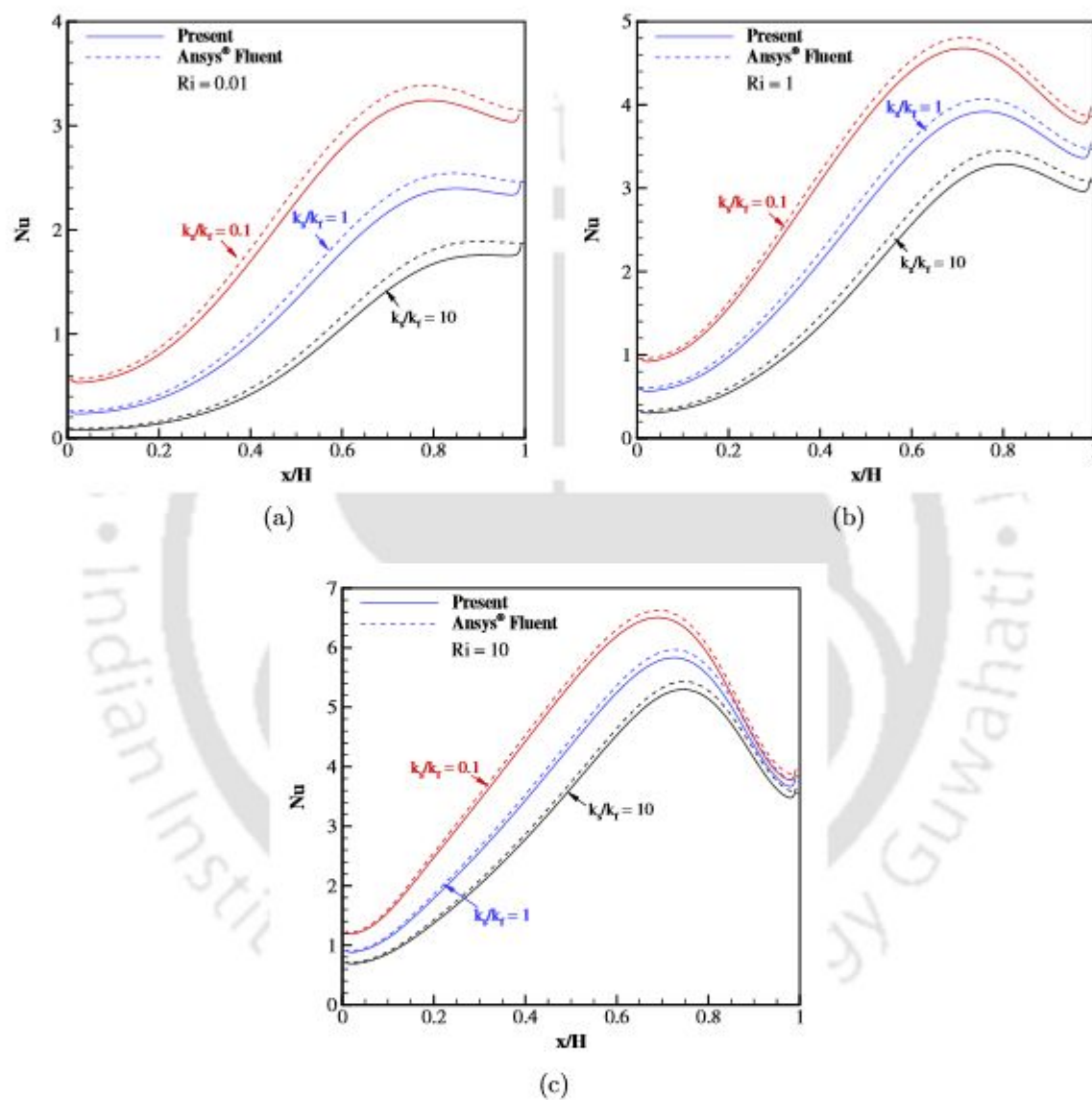


Figure 6.12: Variation of local Nusselt number at the bottom wall of the cavity at different Richardson number and thermal conductivity ratios.

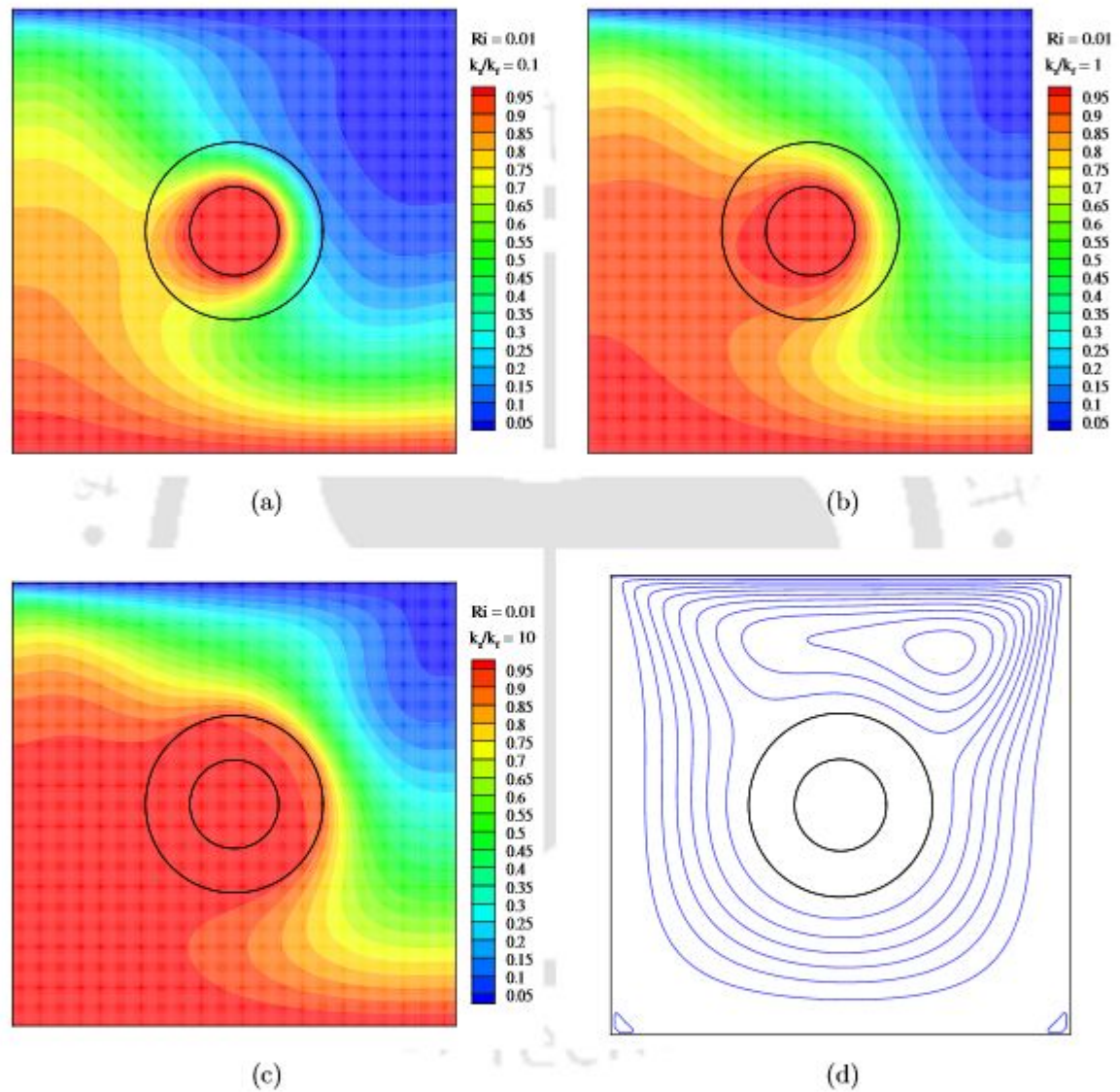


Figure 6.13: Isotherm and streamline contours of mixed convective conjugate heat transfer of non-homogeneous circular cylinder in a lid driven cavity at $Ri = 0.01$ and different thermal conductivity ratios.

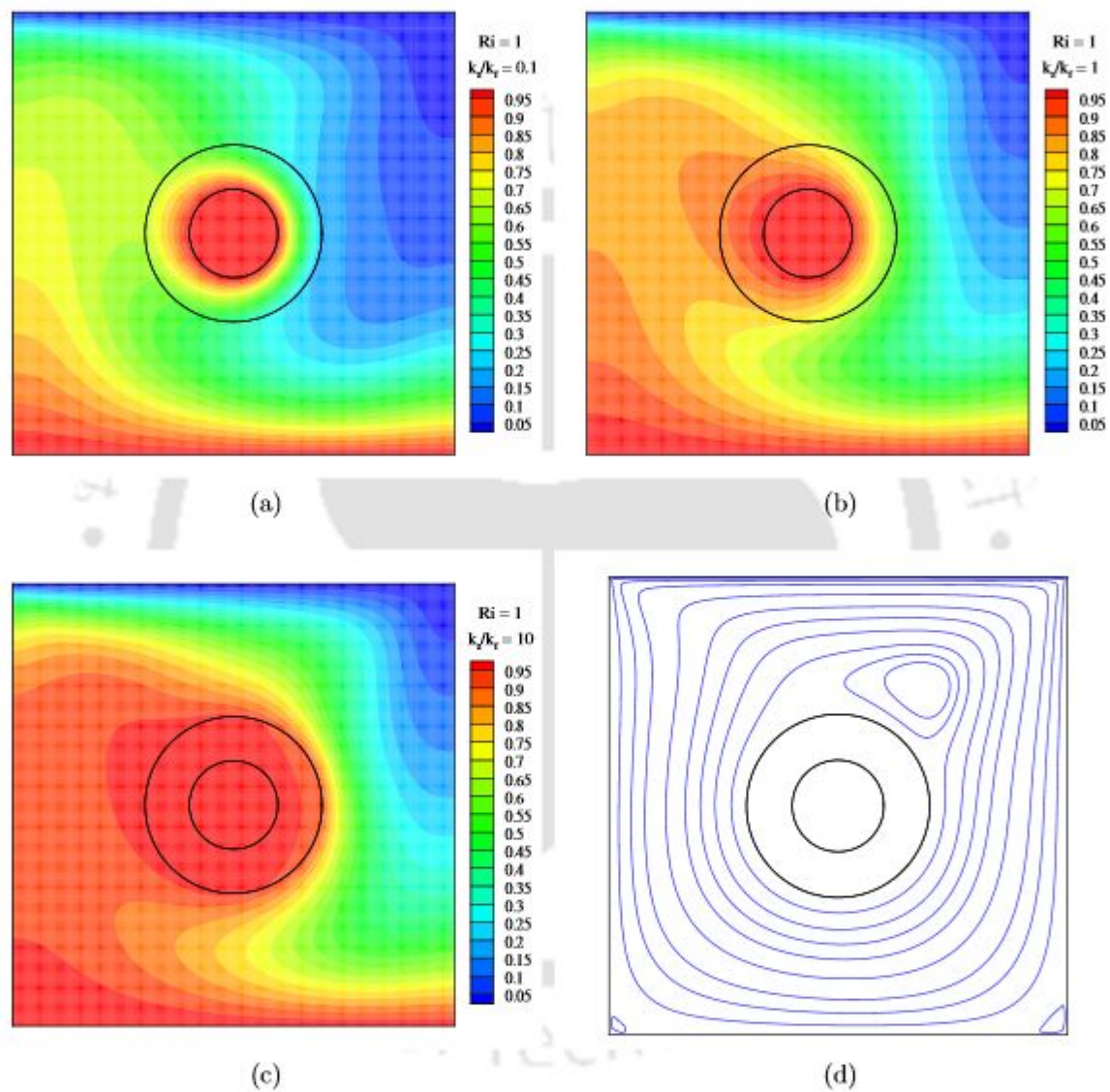


Figure 6.14: Isotherms and streamlines of mixed convective conjugate heat transfer of non-homogeneous circular cylinder in a lid driven cavity at $Ri = 1$ and different thermal conductivity ratios.

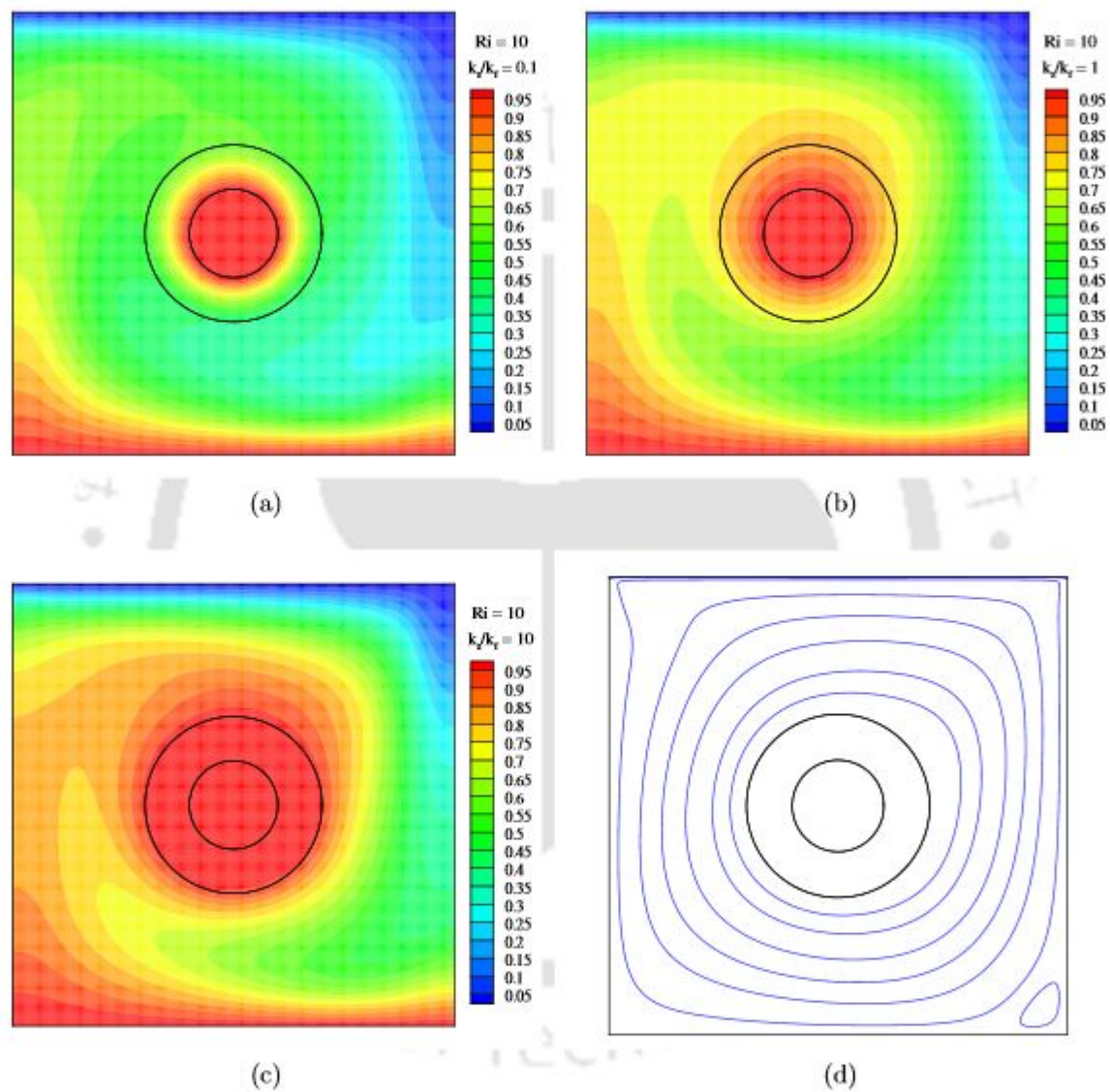


Figure 6.15: Isotherm and streamlines of mixed convective conjugate heat transfer of non-homogeneous circular cylinder in a lid driven cavity at $Ri = 10$ and different thermal conductivity ratios.

6.4 A novel strategy for implementation of adiabatic boundary condition on curved surfaces using PSC

So far, the thesis has established that the present PSC solver can predict complex thermo-fluidic interactions at any complex solid-fluid interface involving different types of convective and conjugate heat transfer problems. However, all of these simulations were subjected to Dirichlet boundary conditions only. The implementation of Neumann and Robin boundary conditions at the immersed surface is impossible with the present class of diffuse-interface IB-LB method. It can be attributed to the fact that the collision operator responsible for implementing boundary conditions, as represented in Eq. 2.31, demands a constant value for the velocity and temperature field. However, the adiabatic boundary condition requires the local temperature gradient ($\partial T/\partial \eta$) to be enforced zero on the surface. The Nu distribution over the cylinder's surface in the preceding sections portrayed that it becomes flat and approaches zero as one decreases the thermal conductivity ratio (k_s/k_f). Furthermore, a closer look into the heat flux continuity condition (Eq. 6.7) at the solid-fluid interface reveals that one can achieve zero temperature gradient $(\partial T/\partial \eta)|_f$ in a limiting sense by opting sufficiently small thermal conductivity ratio (k_s/k_f).

$$\left. \frac{\partial T}{\partial \eta} \right|_f = \frac{k_s}{k_f} \left. \frac{\partial T}{\partial \eta} \right|_s \quad (6.7)$$

In addition, the combination of Eq. 6.3 and Eq. 6.4 does not obligate any constraints for temperature and velocity field. Therefore, these inferences are strategized to implement the adiabatic boundary conditions on an immersed boundary through the present PSC algorithm. The author believes that such an approach has not been forthcoming in the LB literature and is a novel contribution to this community.

In the subsequent sections, the efficacy of the PSC solver for simulating non-trivial benchmark problems involving adiabatic boundary conditions is presented. The benchmark cases are so selected that they encompass a wide variety of heat transfer processes involving pure conduction and natural and mixed convection phenomena.

6.4.1 Purely conductive heat transfer of an adiabatic cylinder inside a cavity

The first test case comprises pure conduction phenomena inside a square cavity of size H , inscribed with an adiabatic circular cylinder of diameter d as depicted in Fig.

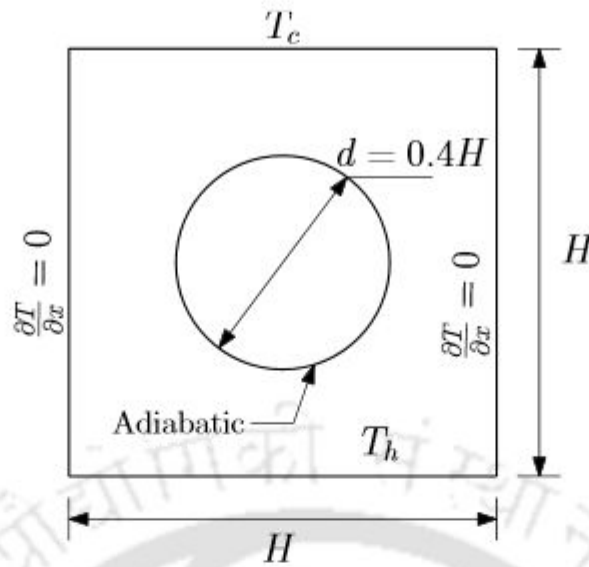


Figure 6.16: Schematic representation of a purely conductive heat transfer of an adiabatic cylinder inside a cavity

6.16. The bottom and top boundaries of the cavity are prescribed higher (T_h) and lower (T_c) temperature, respectively, while the left and right boundaries of the cavity are insulated. Although there are no convection phenomena involved in the present problem, the hydrodynamic PSC evolution equation is solved considering zero fluid velocity for the sake of completeness of the PSC algorithm. Moreover, to maintain the uniformity of notations in the present thesis, let us consider the ratio of thermal conductivity of the circular cylinder to that of the cavity medium to be represented as (k_s/k_f). Apart from it, due to the lack of relevant literature for the present problem, the present solver's data are validated with a commercial finite volume solver, namely Ansys® Fluent. Firstly, it is intended to ensure the limiting value of the thermal conductivity ratio for the proposed scheme. Hence, the thermal conductivity ratios are considered as $k_s/k_f = 10^{-3}, 10^{-4}$ and 10^{-5} in the present problem. Fig. 6.17a shows that the non-dimensional temperature ($\Theta = (T - T_c)/(T_h - T_c)$) distribution over the adiabatic cylinder using all cases of k_s/k_f agrees well with the distribution obtained using Ansys® Fluent. Fig. 6.17b also reveals a good match in local Nu distribution over the heated bottom wall of the cavity between present cases and the Fluent data.

The local rate of heat flux over the cylinder's surface is illustrated in Fig. 6.18a. As expected, the heat flux values are close to zero at most of the cylinder's locations but experience certain, sharp peaks close to the 0° , 90° , 180° and 270° . The highest magnitude of these peaks is experienced by the $k_s/k_f = 10^{-5}$ case. Finally, the isotherms of all the above-mentioned cases are plotted in Figs. 6.18b, 6.18c and 6.18d, in order to select an optimal limiting value of k_s/k_f . It reveals that the $k_s/k_f = 10^{-5}$ condition experiences a greater uniformity in temperature inside the circular cylinder

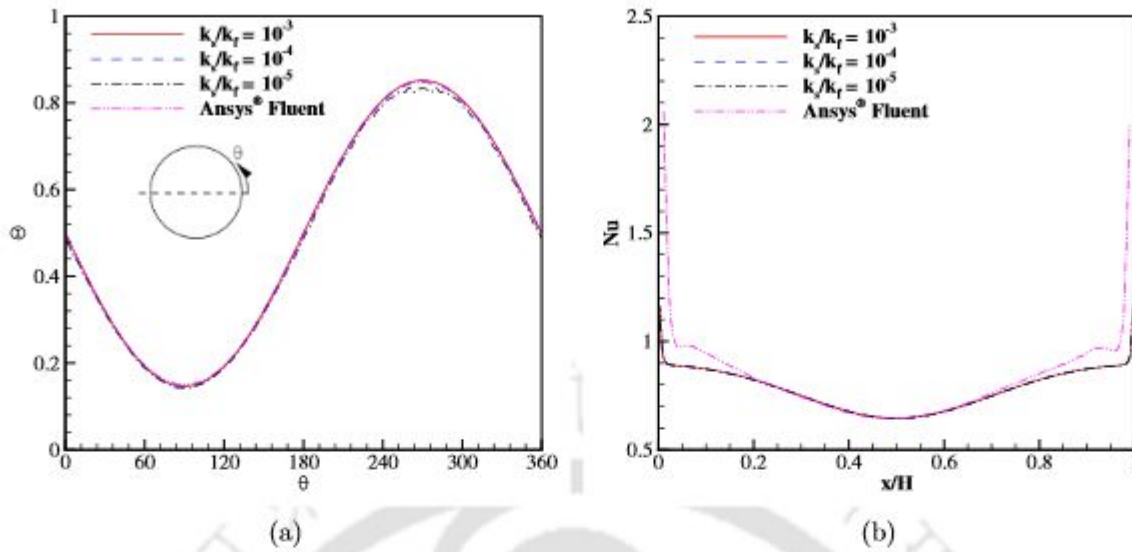


Figure 6.17: (a) Temperature distribution over the adiabatic cylinder's surface at different thermal conductivity ratios and its comparison with Ansys® Fluent. (b) Distribution of local Nusselt number at the heated bottom wall of the cavity at different thermal conductivity ratios.

as compared to the other k_s/k_f cases. Thus, k_s/k_f is selected as 10^{-5} for the rest of the simulations in the present section.

6.4.2 Natural convection of an adiabatic cylinder inside a cavity

The present section investigates the natural convection in a square cavity that is immersed in an insulated circular cylinder. The diameter of the circular cylinder is related to the cavity size as $d = 0.4H$ and depicted in Fig. 6.19. The left and right boundaries of the cavity are provided higher (T_h) and lower (T_c) temperatures, respectively, while the top and bottom boundaries are insulated. The working fluid in the cavity follows the Boussinesq approximation having thermal conductivity k_f and Prandtl number 0.7. Three cases of Rayleigh number are considered in the present study, viz. $Ra = g\beta(T_h - T_c)H^3/(\nu_f \chi_f) = 10^3, 10^4$ and 10^5 . As mentioned in the previous section, the ratio of the thermal conductivity of the circular cylinder to the thermal conductivity of the working fluid is considered as $k_s/k_f = 10^{-5}$. 550×550 lattice nodes are set across the computational domain along with the relaxation time as $\tau_f = 0.6$. In the present study, the data from the commercial finite volume solver Ansys® Fluent is utilized to validate the present solver. Fig. 6.20a depicts that the non-dimensional temperature profile ($\Theta = (T - T_c)/(T_h - T_c)$) over the cylinder's surface is in good agreement with that obtained using the Ansys® Fluent for all cases of Rayleigh

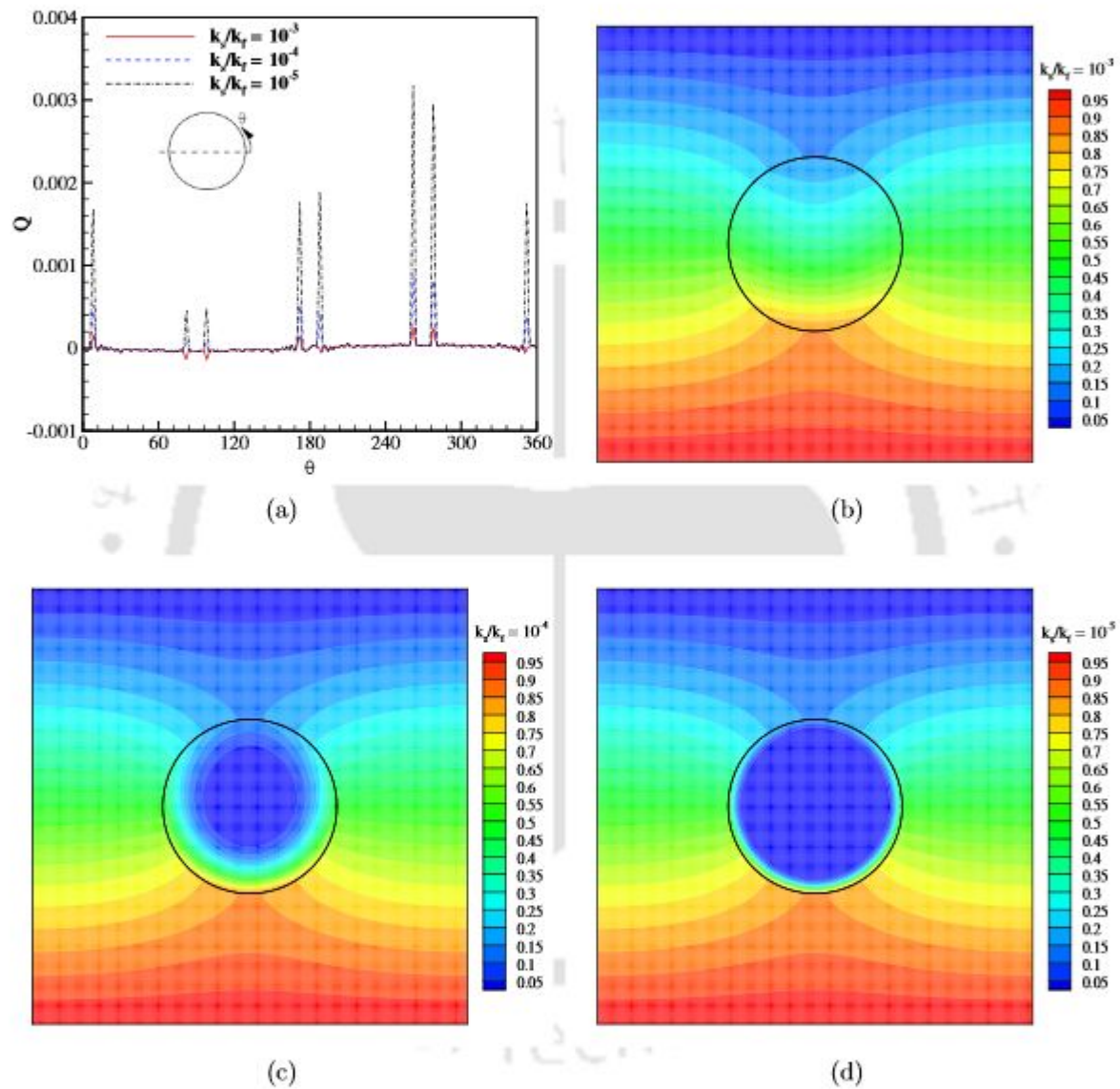


Figure 6.18: (a) Rate of heat flux distribution over the cylinder's surface. (b)-(d) Isotherms of purely conductive heat transfer of an adiabatic cylinder inside a cavity at different thermal conductivity ratios.

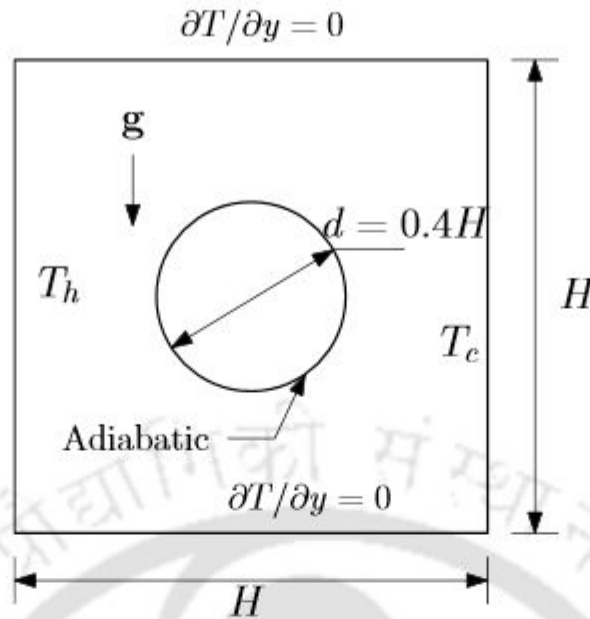


Figure 6.19: Schematic representation of a natural convective heat transfer of an adiabatic cylinder inside a cavity

number considered in this problem. The distribution of local Nusselt number (6.20b) over the heated left boundary of the cavity also agrees well with the data obtained using the Ansys[®] Fluent. Furthermore, the fluid adjacent to the heated wall in the $Ra = 10^5$ case experiences a higher thermal gradient than the others and is evident from the isotherm contours presented in Fig. 6.21.

6.4.3 Mixed convection of an insulated cylinder inside a lid driven cavity

Finally, the efficacy of the proposed methodology is investigated for a mixed convective heat transfer phenomenon in a square cavity around an insulated circular cylinder. Fig. 6.22 shows the schematic representation of the computational setup where a circular cylinder having diameter d is immersed at the geometric center of the square cavity such that $d = 0.4H$, where H represents the size of the square cavity. The bottom and top lid of the cavity are prescribed higher (T_h) and lower (T_c) temperature, respectively, while the left and right boundaries are set insulated. The top lid moves in a horizontal direction with constant velocity (U) such that the Reynolds number is maintained as $Re = UH/\nu_f = 100$. The working fluid inside the cavity follows the Boussinesq approximation and possesses the Prandtl number $Pr = 0.7$. Three Richardson numbers are investigated viz. $Ri = Ra/Re^2 Pr = 0.01, 1$ and 10 which signifies the dominating forced, mixed, and natural convection phenomena, respectively. The data presented in the present section corresponds to the cavity size 500×500 and

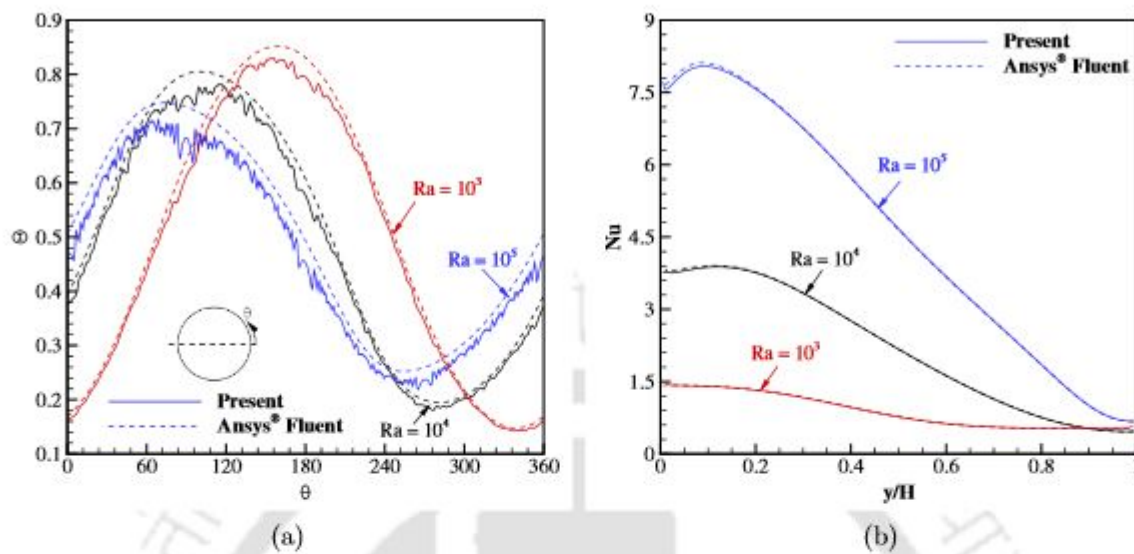


Figure 6.20: (a) Temperature distribution over the adiabatic cylinder's surface at different Rayleigh numbers and its comparison with Ansys® Fluent. (b) Local Nusselt number variation over the heated left wall of the cavity at different Rayleigh numbers.

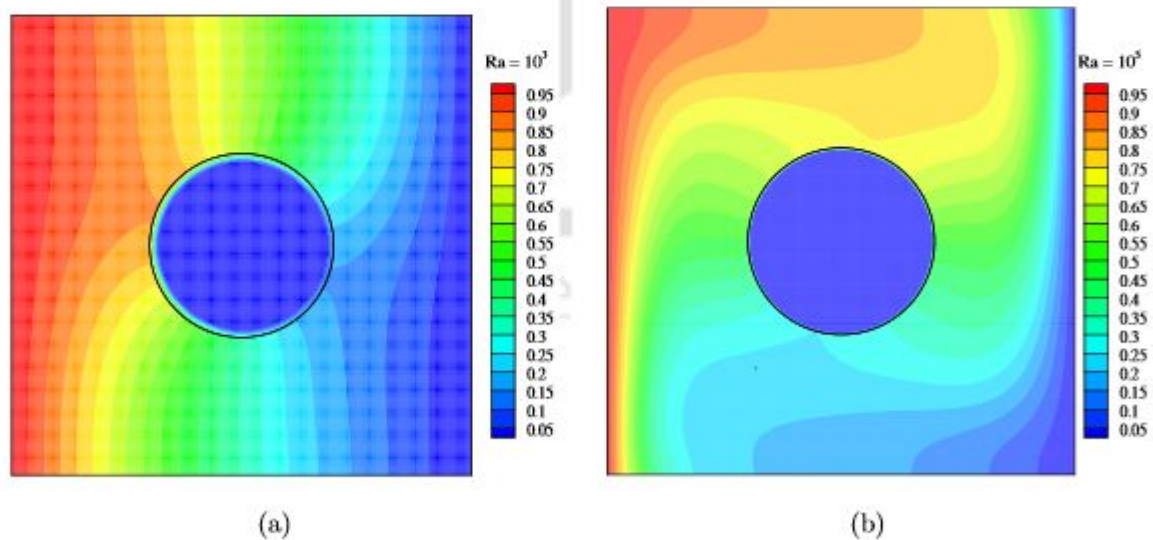


Figure 6.21: Isotherms of natural convective heat transfer of an adiabatic cylinder inside a cavity at (a) $Ra = 10^3$ and (b) $Ra = 10^5$.

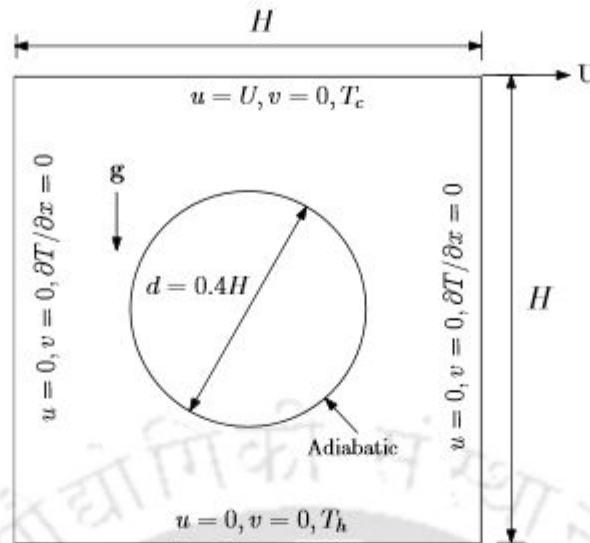


Figure 6.22: Schematic representation of a mixed convective heat transfer of an adiabatic cylinder inside a lid driven cavity

relaxation time $\tau_f = 0.6$.

Fig. 6.23a shows the variation of local heat flux around the cylinder's surface. It is evident from the figure that the computed rate of heat flux around the cylinder is close to zero for most of the cylinder locations. Certain peaks close to angle 0° , 90° , 180° and 270° have magnitude in the order of 10^{-3} , which further decrease with grid refinement. These inferences indicate that the present CHT solver can effectively impose the adiabatic condition on a curved surface. The distribution of non-dimensional temperature profile ($\Theta = T - T_h / T_h - T_c$) for all cases of Ri considered in the present study shows excellent agreement with the distribution obtained by Wang et al. [146]. It further reveals that the temperature distribution varies substantially around the cylinder for $Ri = 1$ and 0.01 while attaining minima around the extreme right position of the cylinder. The minimum temperature shifts to the upper right location of the cylinder for $Ri = 10$ and exhibits relatively smaller variation as compared to the other cases. In addition, the local Nusselt number along the cavity's heated bottom wall and the non-dimensional temperature profiles at location $x/H = 0.15$ agrees well with the literature [118, 146] for all cases of Ri .

The isotherm and streamline contours illustrated in Fig. 6.25 reveal that a large vortex is generated at the upper right part of the cavity at low $Ri = 0.01$ which gradually gets suppressed while one increases Ri to 1 and finally 10. Only a small secondary vortex can be seen at the bottom right corner of the cavity at $Ri = 10$. Owing to the recirculation in the cavity, the temperature close to the left wall is higher than the right wall. Most importantly, the isotherms can be seen perpendicular to the cylinder surface, indicating the accurate implementation of the adiabatic (Neumann)

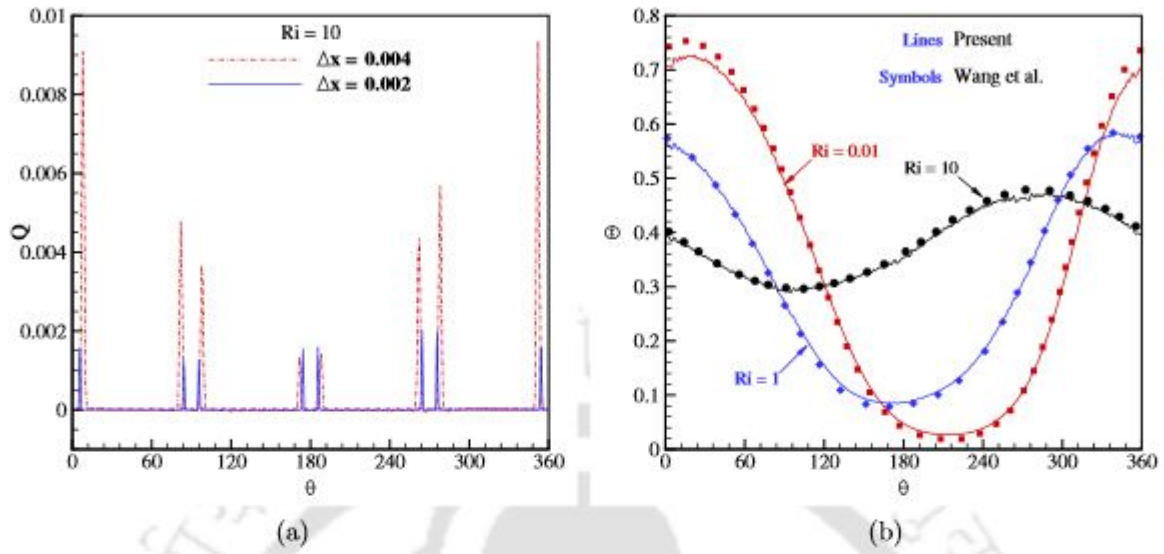


Figure 6.23: (a) Rate of heat flux distribution over the cylinder's surface at different grid resolution. (b) Temperature distribution over an insulated cylinder's surface at different Richardson number and its comparison with Wang et al. [146]. The angle is measured along the clockwise direction starting from the extreme left position of the cylinder.

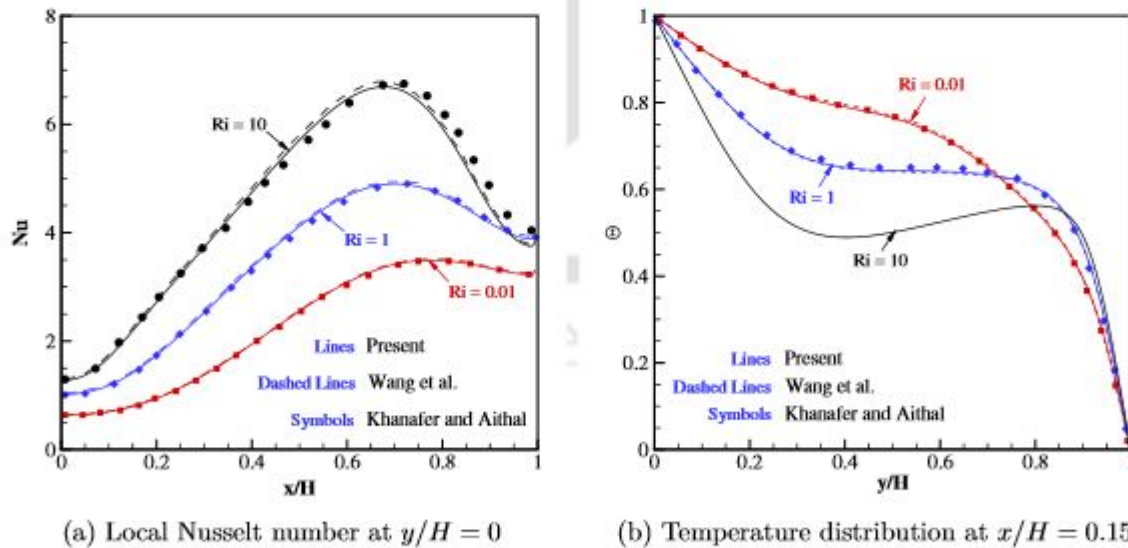


Figure 6.24: (a) Local Nusselt number distribution over the heated bottom wall of the cavity at different Richardson numbers and its comparison with literature [118, 146] (b) Temperature profile inside the cavity at location $x/H = 0.15$ for different Ri and its comparison with the literature [118, 146].

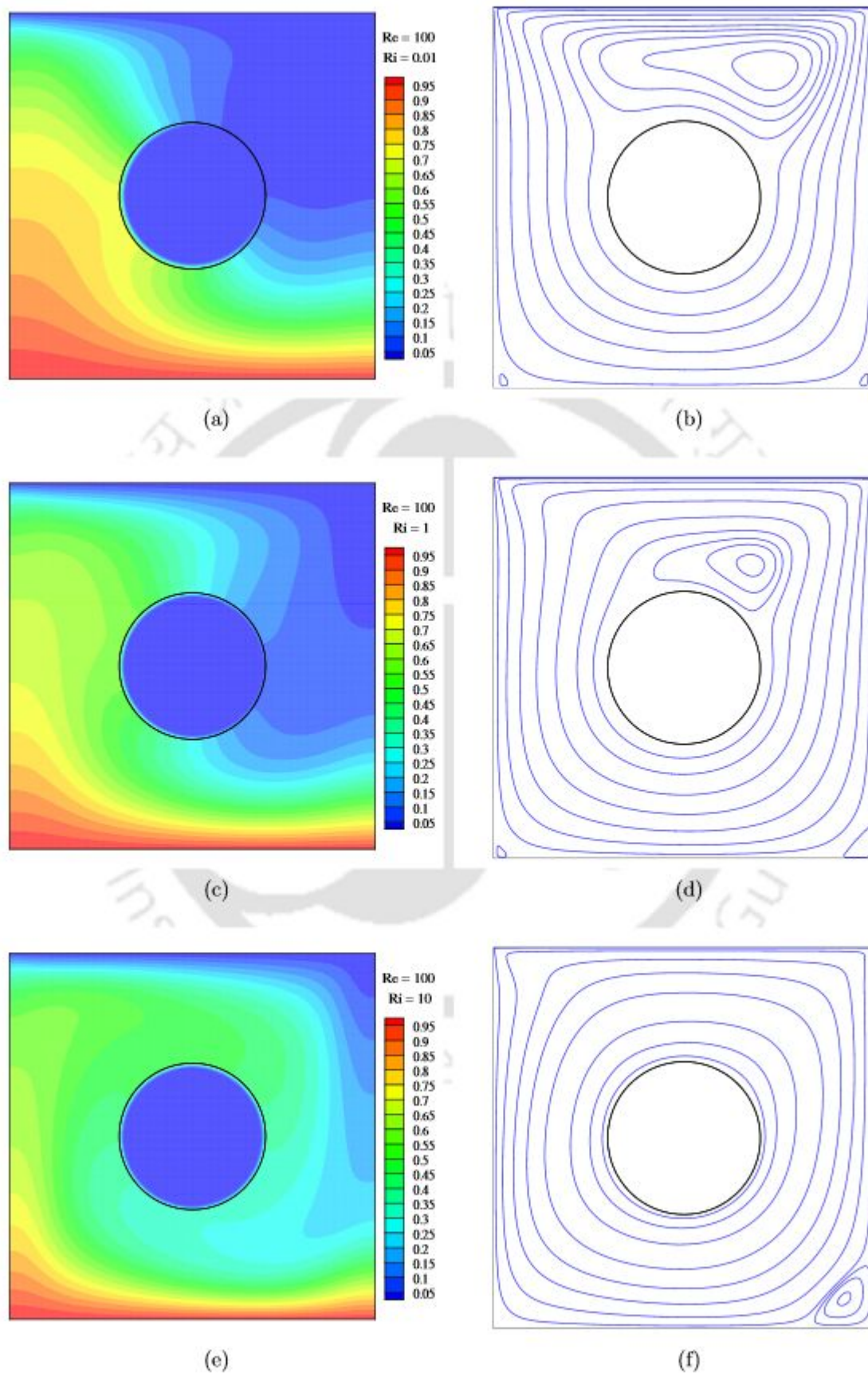


Figure 6.25: Isotherm and streamlines of mixed convective conjugate heat transfer of an insulated circular cylinder in a lid driven cavity for different Richardson numbers. (a-b) $Ri = 0.01$, (c-d) $Ri = 1$ and (e-f) $Ri = 10$

boundary condition on a curved surface.

6.5 Summary

In this chapter, a unified evolution equation for simulating conjugate heat transfer problems has been developed utilizing the partially saturated computational cells (PSC) method. The validation of the solver with respect to a wide range of benchmark problems involving straight and curved boundaries encompassing free, forced, and mixed convection problems indicate the accuracy and robustness of the approach. The approach eliminates any ancillary treatment to the solid-fluid interface while effectively imposing the interfacial boundary conditions. Moreover, severe spurious signals are observed in curved boundary problems, which are inevitable owing to the diffusive nature of the algorithm for interfacial treatment. However, such signals qualitatively follow an accurate trend which can be averaged by passing through a low-pass filter in order to obtain a smoother variation.

It is further observed that the temperature gradient approaches zero around the solid surface while decreasing the solid to fluid thermal conductivity ratio. This inference motivated the author to devise a strategy to implement adiabatic boundary condition at the solid-fluid interface, which hitherto has not been discussed using the PSC methodology in the open literature. The proposed methodology has shown excellent agreement with the reference data when applied to pure conduction, free and mixed convection phenomena.

CHAPTER 7

CONCLUSIONS AND FUTURE SCOPE

“Bring forward what is true. Write it so that it is clear. Defend it to your last breath”

- Ludwig Edward Boltzmann,

This thesis presents the development of an in-house partially saturated cells (PSC) based lattice-Boltzmann solver for thermo-fluidic applications. The key aspects of the thesis comprise a comprehensive assessment of the hydrodynamic and thermal-PSC solver in the purview of accuracy studies, discrete conservation of properties, dependence of spurious fluctuations on grid resolution for moving boundary problems and Galilean invariance. In addition to it the solver’s robustness is demonstrated for a wide range of non-trivial benchmark problems encompassing stationary and moving boundary scenarios for hydrodynamic and thermal flows. The thesis also elucidates the recovery of macroscopic energy equation from the thermal-PSC governing equation through Chapman-Enskog multiscale analysis. A mechanism for the evaluation of local thermal gradients on the curved surfaces is devised for the PSC framework. A comparative analysis is carried out to establish the viability of the PSC method with the conventional DF-IB-LB and DF-IB-TLB methods. Furthermore, a novel algorithm is presented for simulating conjugate heat transfer problems using the PSC methodology. A novel strategy for implementation of adiabatic boundary conditions is also elaborated in the present work. Both of these strategies are validated with standard free, forced and mixed convection problems. The present chapter provides salient inferences of these investigations and draws the directions for future work.

7.1 Major Observations

1. The investigation of spatial order of accuracy for velocity errors reveals that the PSC method is at least first-order accurate for incompressible flows involving moving boundary scenarios. The integrated hydrodynamic quantities also decay linearly with grid refinement. The pressure error, however, exhibits second-order convergence with respect to the grid refinement.
2. The PSC method is approximately discretely conservative in the incompressible limit. The mass conservation errors and the maximum density fluctuations decrease with grid refinement, while both exhibit dependence on the relaxation time (τ_f). The hydrodynamic PSC simulations are recommended at $\tau_f < 1$ for stable computations with negligible compressibility errors.
3. The spurious fluctuations in pressure drag transients in moving boundary problems decay at a rate of 1.67 with grid refinement using PSC methodology.
4. The thermal-PSC algorithm is first-order accurate in space for moving boundary problems, irrespective of the boundary being straight or curved. However, the method is nearly insensitive to the choice of τ_f in straight boundaries, whereas demonstrates an increase in errors with an increase in τ_f in curved boundary problems.
5. The thermal-PSC method exhibits identical distribution of the local Nusselt number (Nu) in moving and stationary reference frames. In addition, the low order of magnitude observed in L_2 -normed difference of local and average Nu indicate the model is Galilean invariant.
6. A thorough analysis of the thermal-PSC algorithm reveals that the present model can estimate the local Nusselt number over curved surfaces with better accuracy for forced and mixed convection problems than the free convection problems. However, with specific advantages and limitations, the present work conclusively demonstrates the efficacy and robustness of the thermal-PSC algorithm for incompressible thermal flows.
7. The linear decay of velocity and temperature errors with grid refinement using PSC is comparable to the decay at similar rate using the conventional DF-IB-LB method. The pressure error exhibits quadratic spatial convergence for both methodologies.
8. The PSC method exhibits an increase in velocity and temperature errors with the increase in τ_f . On the contrary, the DF-IB-LB approach experiences a decrease

in velocity and temperature errors until $\tau_f = 1.5$ and 1.6, respectively, beyond which they exhibit an increasing trend. The pressure errors, however, carry identical magnitude of errors and increase with increasing τ_f .

9. The magnitude of local maximum divergence using the PSC are found to be lower than the DF-IB-LB approach in the hydrodynamic simulations. In addition, the mass flux errors and maximum density fluctuations decay with grid refinement, while exhibit an increasing trend with increase in τ_f using both methodologies.
10. The PSC method produces a smoother signal in pressure drag transient as compared to the DF-IB-LB approach. Furthermore, these methods unveil identical hydrodynamic and thermal characteristics in moving and stationary reference frames, indicative of the methods being Galilean invariant.
11. The proposed PSC-based solver for simulating conjugate heat transfer (CHT) problems reveals excellent agreement in predicting heat transfer characteristics with respect to the reference data. It is benchmarked with non-trivial test cases involving free, forced and mixed convection problems encompassing low to high thermal conductivity ratios.
12. An important inference from the CHT study that the temperature gradient approaches zero around the solid-fluid interface while decreasing the solid to fluid thermal conductivity ratio, led to the development of a novel strategy for implementation of adiabatic boundary condition using the PSC approach. It is observed that the thermal conductivity ratio in the order of 10^{-5} produces desirable effect towards achieving an insulated surface condition. Finally, the proposed technique is benchmarked for establishing its robustness and accuracy by simulating non-trivial test cases like pure conduction, free and mixed convection problems.

With specific advantages and limitations, the present thesis endorses that the PSC methodology possesses an enormous potential for simulating complex and moving boundary thermo-hydraulic applications as comparable to the conventional IB-LB solvers.

7.2 Major contributions

The major contributions of the thesis which have hitherto not been presented in open literature are enlisted as follows

- Studies on key aspects of numerical appraisal of the hydrodynamic-PSC algorithm like accuracy, discrete conservation of properties and spurious force oscillations in moving boundary problems. Besides, benchmarking the solver for a wide range of stationary and moving boundary problems.
- Studies on the accuracy and Galilean invariance of the thermal-PSC algorithm. Benchmarking the solver for a broad spectrum of thermal flows involving free, forced and mixed convection encompassing stationary and moving boundary scenarios.
- Development of a novel formulation for simulating conjugate heat transfer process based on the PSC algorithm.
- A novel strategy for implementation of adiabatic boundary conditions on curved surfaces using the PSC approach.

7.3 Directions for future research

In view of the development of the PSC solver carried out in the present thesis, one can infer that several important aspects of numerical appraisal have been discussed in both hydrodynamic and thermal front. However, challenging applications like two-dimensional vortex-induced-vibrations, etc., need to be taken up in future to clearly highlight the limitations and advantages of the method. Additionally, some of the possible directions for immediate explorations in near future are elaborated below.

- Spatial order of accuracy of the PSC model: The present thesis shows that the spatial order of accuracy of the PSC solver is first-order. The accuracy improvement of any LB solver is not straightforward as it involves several sources of errors [120]. However, the quest for such improvement would necessitate some mathematical intervention of the existing evolution equations. Primarily, the solid collision operator of the PSC model, responsible for accurately implementing the boundary conditions, could be targeted for determining the factors contributing to the accuracy improvement. Although the Chapman-Enskog multiscale analysis for PSC models presented by Najuch and Sun [49] yields extraneous error terms in the recovered macroscopic N-S equations but fails to provide specific guidelines for its accuracy improvement. Nevertheless, the Taylor series analysis of the LB model presented by Holdych et al. [147] yields truncation and compressibility error terms as a function of relaxation time, grid size, and temporal size. A similar analysis of the PSC evolution equation would be helpful to de-

termine definite terms responsible for the lower order of accuracy and eventually guide toward developing modified collision operators with improved accuracy.

- Mitigation of artificial slip velocity and temperature jump: The artificial slip velocity and temperature jump at the solid-fluid boundary are inevitable in any diffuse-interface IB-LB method owing to its diffuse nature and discontinuity in the velocity [124] and temperature gradient [73] while implementing the boundary conditions. However, the severity of such hydrodynamic and thermal slip can be mitigated by identifying tunable key parameters through a rigorous analysis of the density distribution function as presented in literature [65, 148]. A similar analysis for PSC models would be beneficial to recognize key tunable parameters which can reduce the severity of the artificial slip and eventually improve its accuracy.
- Development of a PSC-based multiphase solver: The present PSC solver can be coupled with multiphase models to simulate complex thermo-fluidic interaction of multiphase flows with irregular structures. The development of an accurate PSC model which can simultaneously predict the interfacial forces and efficiently track the solid-fluid interface would be an essential contribution to the LB community.
- Implementation of Neumann and Robin-type boundary conditions: The implementation of Neumann and Robin-type boundary conditions is not feasible using the present PSC models owing to the requirement of constant velocity and temperature values in the solid collision operator for the implementation of boundary conditions. However, a deeper understanding of these models to overcome the limitation of handling only Dirichlet-type boundary conditions is necessary for broadening the scope of this approach.

Appendix A

In this section we intend to recover the macroscopic energy equation from thermal-PSC equation via Chapman-Enskog analysis. In the remainder of the analysis, we would use Einstein notations and use shorter notations for expressing partial derivatives like $\frac{\partial}{\partial x} = \partial_x$ and $\frac{\partial}{\partial t} = \partial_t$ for brevity. Distribution functions will be henceforth, written as $g_i(\mathbf{x}, t) = g_i$, and $g_i^{eq}(\rho_f, \mathbf{U}_p, T_p) = g_i^{eq}(\rho_f, U_{p,\alpha}, T_p)$ for readability. Thermal-PSC Eq. (2.30) can be rearranged as

$$g_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - g_i(\mathbf{x}, t) = \Psi_i^{BGK} + Q_i(\mathbf{x}, T, \mathbf{u}, t) \quad (7.1)$$

where, $Q_i(\mathbf{x}, T, \mathbf{u}, t) = -\sum_S B_t(\mathbf{x}, \tau_{g,f}) \Psi_i^{BGK} + \sum_S B_t(\mathbf{x}, \tau_{g,f}) \Psi_i^B$.

The expression for Q_i using Eq. (2.31) can be expressed as,

$$Q_i(\mathbf{x}, t) = \sum_s B_t(\mathbf{x}, \tau_{g,f}) \left\{ \frac{\Delta t}{\tau_{g,f}} [g_i(\mathbf{x}, t) - g_i^{eq}(\rho_f, \mathbf{u}, T)] - g_{-i}(\mathbf{x}, t) - g_i(\mathbf{x}, t) + g_i^{eq}(\rho_f, \mathbf{U}_p, T_p) + g_{-i}^{eq}(\rho_f, \mathbf{u}, T) \right\} \quad (7.2)$$

The perturbation ansatz for energy distribution function (g_i), spatial and temporal derivatives and source term is given as

$$g_i = g_i^{(0)} + \epsilon g_i^{(1)} + \epsilon^2 g_i^{(2)} + \dots \quad (7.3a)$$

$$\partial_t = \epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} + \epsilon^3 \partial_t^{(3)} + \dots \quad (7.3b)$$

$$\partial_\alpha = \epsilon \partial_\alpha^{(1)} \quad (7.3c)$$

$$Q_{i,\alpha} = \epsilon Q_{i,\alpha}^{(1)} + \epsilon^2 Q_{i,\alpha}^{(2)} \quad (7.3d)$$

ϵ signifies a small parameter that represents Knudsen number. Applying Taylor series expansion to Eq. (7.1) and some algebra yields

$$\begin{aligned} & \Delta t \left(\partial_t + c_{i,\alpha} \partial_\alpha \right) g_i + \mathcal{O}(\Delta t^3) \\ &= \Psi_i^{BGK} + Q_{i,\alpha} - \frac{\Delta t}{2} \left(\partial_t + c_{i,\alpha} \partial_\alpha \right) \left(\Psi_i^{BGK} + Q_{i,\alpha} \right) \end{aligned} \quad (7.4)$$

where, higher order terms than $\mathcal{O}(\Delta t)^3$ are neglected. Applying multiscale expansion

(Eqs. 7.3), to the above equation gives ϵ^0, ϵ and ϵ^2 -order equations as follows

$$\mathcal{O}(\epsilon^0) : g_i^{(0)} = g_i^{eq}(\rho_f, u_\alpha, T) \quad (7.5)$$

$$\mathcal{O}(\epsilon) : \left[\partial_t^{(1)} + c_{i,\alpha} \partial_\alpha^{(1)} \right] g_i^{(0)} = -\frac{g_i^{(1)}}{\tau_{g,f}} + \frac{Q_{i,\alpha}^{(1)}}{\Delta t} \quad (7.6)$$

$$\begin{aligned} \mathcal{O}(\epsilon^2) : \partial_t^{(2)} g_i^{(0)} + \left(1 - \frac{\Delta t}{2\tau_{g,f}} \right) \left[\partial_t^{(1)} + c_{i,\alpha} \partial_\alpha^{(1)} \right] g_i^{(1)} = \\ -\frac{g_i^{(2)}}{\tau_{g,f}} + \frac{Q_{i,\alpha}^{(2)}}{\Delta t} - \frac{1}{2} \left(\partial_t^{(1)} + c_{i,\alpha} \partial_\alpha^{(1)} \right) Q_{i,\alpha}^{(1)} \end{aligned} \quad (7.7)$$

From Eq. (7.6) we get,

$$g_i^{(1)} = \tau_{g,f} \left[\frac{Q_{i,\alpha}^{(1)}}{\Delta t} - \left(\partial_t^{(1)} + c_{i,\alpha} \partial_\alpha^{(1)} \right) g_i^{(0)} \right] \quad (7.8)$$

Substituting Eq. (7.8) into Eq. (7.7) yields $\mathcal{O}(\epsilon^2)$ equation as

$$\begin{aligned} \partial_t^{(2)} g_i^{(0)} - \left(\tau_{g,f} - \frac{\Delta t}{2} \right) \left[\partial_t^{(1)} + c_{i,\alpha} \partial_\alpha^{(1)} \right]^2 g_i^{(0)} \\ = -\frac{g_i^{(2)}}{\tau_{g,f}} + \frac{Q_{i,\alpha}^{(2)}}{\Delta t} - \frac{\tau_{g,f}}{\Delta t} \left(\partial_t^{(1)} + c_{i,\alpha} \partial_\alpha^{(1)} \right) Q_{i,\alpha}^{(1)} \end{aligned} \quad (7.9)$$

The 0th and 1st moment of $\mathcal{O}(\epsilon^0)$ equation yield respectively as,

$$\sum_i g_i^{(0)} = \rho_f T \quad (7.10)$$

$$\sum_i g_i^{(0)} c_{i,\alpha} = \rho_f u_\alpha T \quad (7.11)$$

Thus, 0th moment of $\mathcal{O}(\epsilon)$ equation can be expressed on the time scale $t^{(1)} = \epsilon t$ as

$$\partial_t^{(1)} T + u_\alpha \partial_\alpha^{(1)} T = \sum_i \frac{Q_{i,\alpha}^{(1)}}{\rho_f T} \quad (7.12)$$

From 1st moment of $\mathcal{O}(\epsilon)$ equation, we obtain

$$\sum_i g_{i,\alpha}^{(1)} c_{i,\alpha} = -\tau_{g,f} \left[\partial_t^{(1)} (\rho_f u_\alpha T) + \partial_\beta^{(1)} \left(\frac{2}{3} \rho_f c^2 T \right) - \frac{\sum_i Q_{i,\alpha}^{(1)} c_{i,\alpha}}{\Delta t} \right] \quad (7.13)$$

Table A: Moments of perturbed expansions of Q_i

	$Q_i^{(1)}$	$Q_i^{(2)}$
$\sum_i Q_{i,\alpha}^{(n)}$	$\sum_S B_t \rho_f (T_p - T)$	0
$\sum_i Q_{i,\alpha}^{(n)} c_{i,\alpha}$	$\sum_S B_t \rho_f (U_{p,\alpha} T_p - u_\alpha T)$	0

And, the 2^{nd} term at LHS of Eq. (7.9) alongwith the constraint $\sum_i g_i^{(n)} = 0$ for $n \geq 1$ can be rewritten as

$$\begin{aligned} \sum_i \left(\partial_t^{(1)} + c_{i,\alpha} \partial_\alpha^{(2)} \right)^2 g_i^{(0)} &= \partial_t^{(1)} \sum_i \frac{Q_{i,\alpha}^{(1)}}{\Delta t} - \frac{1}{\tau_{g,f}} \partial_\alpha^{(1)} \sum_i g_{i,\alpha}^{(1)} c_{i,\alpha} \\ &\quad + \frac{1}{\Delta t} \partial_\alpha^{(1)} \sum_i Q_{i,\alpha}^{(1)} c_{i,\alpha} \end{aligned} \quad (7.14)$$

Thus, putting Eq. (7.13) into Eq. (7.14) yields

$$\begin{aligned} \sum_i \left(\partial_t^{(1)} + c_{i,\alpha} \partial_\alpha^{(2)} \right)^2 g_i^{(0)} &= \partial_t^{(1)} \sum_i \frac{Q_{i,\alpha}^{(1)}}{\Delta t} + \frac{2}{3} \nabla^{(1)2} T \rho_f c^2 \\ &\quad + \mathcal{O}(u^2 T) \end{aligned} \quad (7.15)$$

Hence, 0^{th} moment of $\mathcal{O}(\epsilon^2)$ equation is expressed on the time scale $t^{(2)} = \epsilon^2 t$ as

$$\begin{aligned} \partial_t^{(2)} T &= \chi \nabla^{(1)2} T + \sum_i \frac{Q_{i,\alpha}^{(2)}}{\rho_f \Delta t} - \frac{1}{2\rho_f} \partial_t^{(1)} \sum_i Q_{i,\alpha}^{(1)} \\ &\quad - \frac{\tau_{g,f}}{\rho_f \Delta t} \partial_\alpha^{(1)} \sum_i Q_{i,\alpha}^{(1)} c_{i,\alpha} \end{aligned} \quad (7.16)$$

Eq. (7.16) gives us the relation of thermal diffusivity (χ) as a function of non-dimensional relaxation time ($\tau_{g,f}$) which is already expressed in Eq. (2.10). Now, multiplying Eq. (7.12) with ϵ and Eq. (7.16) with ϵ^2 and adding them while reversing the perturbation we obtain,

$$\begin{aligned} \frac{\partial T}{\partial t} + u_\alpha \partial_\alpha T &= \chi \nabla^2 T + \frac{1}{\Delta t} \left[\epsilon \sum_i \frac{Q_{i,\alpha}^{(1)}}{\rho_f} + \epsilon^2 \sum_i \frac{Q_{i,\alpha}^{(2)}}{\rho_f} \right] \\ &\quad - \epsilon^2 \frac{1}{2\rho_f} \partial_t^{(1)} \sum_i Q_{i,\alpha}^{(1)} - \epsilon^2 \frac{\tau_{g,f}}{\rho_f \Delta t} \partial_\alpha^{(1)} \sum_i Q_{i,\alpha}^{(1)} c_{i,\alpha} \end{aligned} \quad (7.17)$$

The summary of moments of perturbed expansions of Q_i are listed in table A. Thus, using moments listed in table A, Eq. (7.17) can be rewritten as

$$\begin{aligned}
\frac{\partial T}{\partial t} + u_\alpha \partial_\alpha T = & \chi \nabla^2 T + \frac{1}{\Delta t} \left[\epsilon \sum_S B_t (T_p - T) \right] \\
& - \frac{\epsilon^2}{2} \partial_t^{(1)} \left[\sum_S B_t (T_p - T) \right] - \frac{\epsilon^2}{\Delta t} \tau_{g,f} \partial_\alpha^{(1)} \sum_S B_t [U_{p,\alpha} T_p - u_\alpha T]
\end{aligned} \tag{7.18}$$

For Dirichlet boundary condition, above equation becomes

$$\begin{aligned}
\frac{\partial T}{\partial t} + u_\alpha \partial_\alpha T = & \chi \nabla^2 T + \frac{1}{\Delta t} \left[\epsilon \sum_S B_t (T_p - T) \right] \\
& + \frac{\epsilon^2}{2} \sum_S B_t \partial_t^{(1)} T + \frac{\epsilon^2}{\Delta t} \tau_{g,f} \sum_S B_t \partial_\alpha^{(1)} (u_\alpha T)
\end{aligned} \tag{7.19}$$

Thus, the macroscopic energy equation is recovered from the thermal-PSC evolution equation. It is to be noted here that, 2nd term onwards in the RHS of Eq. (7.19) represent error terms which may dictate temperature jump at the solid-fluid interface.

PUBLICATIONS

Journals

1. S. Majumder, A. Ghosh, D. N. Basu and G. Natarajan, **"Re-examining the partially saturated-cells method for incompressible flows with stationary and moving bodies"**, *Computers and Mathematics with Applications*, vol. 110, pp. 19–39, 2022. <https://doi.org/10.1016/j.camwa.2022.01.034>
2. S. Majumder, A. Ghosh, D. N. Basu and G. Natarajan, **Computational assessment of immersed boundary–lattice Boltzmann method for complex moving boundary problems**. *Computational Particle Mechanics*, (2022) <http://doi.org/10.1007/s40571-022-00487-5>
3. S. Majumder, D. N. Basu and G. Natarajan, **Comprehensive assessment of the Partially-Saturated-Cells framework for convective problems**. (submitted)
4. S. Majumder, D. N. Basu and G. Natarajan, **A novel diffuse interface immersed-boundary lattice-Boltzmann method for complex boundary conjugate heat transfer problems**. (under preparation)
5. S. Majumder, D. N. Basu and G. Natarajan, **A short note on the implementation of adiabatic boundary conditions using partially saturated cells method**. (under preparation)

Conference proceedings

1. A. Ghosh, S. Majumder, D. N. Basu and G. Natarajan, **Comparative study of two immersed boundary approaches in the Lattice Boltzmann Framework**, *Proceedings of the 7th International and 45th National Conference on Fluid Mechanics and Fluid Power (FMFP)*, IIT Bombay, (2018).
2. S. Majumder, A. Ghosh, D. N. Basu and G. Natarajan, **Development of an immersed boundary-thermal lattice Boltzmann solver for fluid-particle interaction in energy management systems**, *IOP Conference Series: Earth and Environmental Science* 463, 012044, (2020).

3. S. Majumder, A. Ghosh, D. N. Basu and G. Natarajan, **Computational assessment of immersed boundary-lattice Boltzmann method for complex moving boundary problems**, *Proceedings of the 8th International and 47th National Conference on Fluid Mechanics and Fluid Power (FMFP)*, IIT Guwahati, (2020).
4. S. Majumder, D. N. Basu and G. Natarajan, **Development and validation of a novel solid collision operator in IB-LB framework for simulation of thermal flows**, *7th International Heat Transfer Conference*, South Africa, (2023) (accepted).
5. S. Majumder, D. N. Basu and G. Natarajan, **Comparative appraisal of direct-forcing immersed-boundary lattice-Boltzmann method and partially saturated cells method for thermofluidic applications**, *International Conference on Heat and Mass Transfer*, Germany, (2023) (accepted).



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