Chapter 1

Introduction

1.1 Background

The behaviour of fluids, such as gases and liquids, under different conditions is studied in the field of fluid dynamics. Solutions of fluid flow problems provide insights into the characteristic of fluids in motion or at rest. The study and analysis of flow problems enable us to develop efficient designs, predict the performance of fluid systems, and address challenges in diverse fields. We may enhance technology, investigate natural occurrences, and enhance our understanding of the world around us by examining the complexities of fluid movement. Both ordinary differential equations and partial differential equations govern a large number of physical systems that deal with fluid behaviour. Among various governing equations, the system of Navier-Stokes (N-S) equations stand as a keystone of fluid dynamics, providing a mathematical framework for comprehending fluid phenomena. The N-S equations are derived from fundamental ideas like Newton's second law of motion and the conservation of mass. The unsteady N-S equations in nondimensional primitive variables (u, v, p) can be written as

$$\begin{cases} \nabla \cdot \mathbf{u} = 0, & (1.1a) \\ \dfrac{\partial \mathbf{u}}{\partial t} = -\left(\mathbf{u} \cdot \nabla\right)\mathbf{u} - \nabla p + \dfrac{1}{Re}\Delta \mathbf{u} + \boldsymbol{\ell}, & (1.1b) \end{cases}$$

where $\mathbf{u}$ denotes the velocity vector, p is the pressure, t is the time and $\boldsymbol{\ell}$ is the body force. All lengths and velocities present in equation (1.1) are nondimensionalized with respect to the characteristic velocity U_∞ and characteristic length L respectively. Thus $Re = U_\infty L/\nu$, where ν is the kinematic viscosity. Though equation (1.1) represents the fluid flow phenomena accurately, a traditional difficulty lies in the lack of pressure boundary condition. To alleviate this challenge, an alternative formulation economical in two dimension (2D) which includes streamfunction (ψ) and vorticity (ω) is used. This formulation is often referred to as streamfunction-vorticity ($\psi - \omega$) formulation and is written as

$$\begin{cases} \dfrac{\partial \omega}{\partial t} = -\mathbf{u}\cdot\nabla\omega + \dfrac{1}{Re}\nabla^2\omega, & (1.2\text{a}) \\ \nabla^2\psi = -\omega, & (1.2\text{b}) \end{cases}$$

where $\omega = (\nabla \times \mathbf{u})\cdot\hat{k}$ is the out-of-plane component of vorticity and $\mathbf{u} = \nabla \times \Psi$ with $\Psi = (0, 0, \psi)$.

In large number of physical situations and applications, for instance insulation of nuclear reactors, solar energy collection, air conditioning of rooms, crystal growth of liquids, cooling of electronic equipment etc., buoyancy and temperature driven flows play a vital role. Because of the diversified use, these physical situations provide a fundamental importance in understanding the buoyancy driven flows. Contrary to convective and diffusive transport of unknown variables, in these systems heat transfer in temperature driven flows are investigated. The governing equation for these problems is the unsteady nondimensional form of the system of Boussinesq equations, derived by linearizing the N-S equations and applying the Boussinesq approximation which is written as

$$\begin{cases} \dfrac{\partial \omega}{\partial t} = -\mathbf{u}\cdot\nabla\omega + Pr\nabla^2\omega + RaPr\dfrac{\partial \mathscr{T}}{\partial x} + \boldsymbol{f}, & (1.3\text{a}) \\ \nabla^2\psi = -\omega, & (1.3\text{b}) \\ \dfrac{\partial \mathscr{T}}{\partial t} = -\mathbf{u}\cdot\nabla\mathscr{T} + \nabla^2\mathscr{T}, & (1.3\text{c}) \end{cases}$$

where $\mathscr{T}$ denotes the dimensionless temperature, Pr and Ra stand for Prandtl number and Rayleigh number respectively. The Rayleigh number is a dimensionless quantity defined as $Ra = \dfrac{g\beta\delta\mathscr{T}L^3}{\kappa\nu}$, where β is the coefficient of thermal expansion of the fluid, g is the acceleration due to gravity, $\delta\mathscr{T}$ is the temperature difference, L is the length, κ is the thermal diffusivity and ν is the kinematic viscosity of the fluid.

An equation that is often used as prototype equation to describe the equations (1.1)–(1.3) is the convection-diffusion equation (CDE). In a convex domain Ω with its boundary $\partial\Omega$ the CDE in conservative form for $\phi \in \Omega$ is described as

$$a\frac{\partial \phi}{\partial t} - \nabla \cdot (\boldsymbol{D}\nabla\phi) + \nabla \cdot (\boldsymbol{C}\phi) = s \tag{1.4}$$

which is supplemented with the necessary boundary condition

$$\phi = \phi^b \text{ on } \partial\Omega. \tag{1.5}$$

In equation (1.4), $a > 0$ is a constant; $\boldsymbol{C}$ is the convection vector and $\boldsymbol{D}$ diffusion matrix; and s is the forcing function. The unknown transport variable ϕ, forcing function s along with the coefficient functions in $\boldsymbol{C}$ and $\boldsymbol{D}$ are assumed to have sufficient smoothness in Ω. This is to mention here that all the steady equations can be represented by the steady form of CDE which is obtained by omitting the temporal derivative term.

The coupled nonlinear PDEs like N-S equations, Boussinesq equations possess analytic solutions only under simplifying assumptions. Thus, in majority of the physical situations, one has to enforce numerical methods to solve these equations. This idea of adopting numerical techniques and algorithms to solve the fluid flow problems is often known as Computational Fluid Dynamics. The noteworthy advancement in computer architecture has made dealing with complex fluid flow situations possible. Among various approaches that has been employed in Computational Fluid Dynamics over the years, one can cite Finite Difference Methods (FDM), Finite Element Methods (FEM) and Finite Volume Methods (FVM). The FDM is found to be most extensively used for the solution in thes computational domain due to its ease of application. The fundamental methodology, in FDM, entails discretizing the problem domain by employing a ordered grid and estimating the gradients that appear in the governing equations using difference formula at each nodes. This approximation produces a system of linear equations which can subsequently be solved using a matrix solution technique.

By employing the Taylor series expansion of the variables at the grid points, the most common finite difference approximations of the derivatives are determined.

The efficiency of these schemes is assessed based on the leading term in the truncation error of this expansion. For example, a difference method is considered to be accurate up to the order m, abbreviated as $\mathcal{O}(h^m)$, when the corresponding truncation error is proportional to h^m asymptotically, h being the fixed grid spacing. Being very simple and convenient to use, $\mathcal{O}(h^2)$ central difference schemes have been a preferred method for formulating discrete approximations for linear partial differential equations (PDE). If the solutions obtained by these methods behave properly, they are known to produce fairly acceptable results on feasible meshes. But, if the mesh is not sufficiently finer for some situations, such as those with higher values of Re and Ra, the solution may exhibit physically absurd behavior. However, mesh refining always introduces more nodes into the system, increasing the system size hereby requiring more CPU time and computer memory. Additionally, the bandwidth of the coefficient matrix is increased by the traditional higher-order accurate approximation of the gradients at the nodes, which results in an expanded stencil. Greater arithmetic operations are the end effect of both mesh refinement and greater matrix bandwidth. Thus neither a lower-order accurate approach on a fine mesh nor a higher-order accurate one on a noncompact stencil is computationally efficient. As a result, it is desirable to develop methods that are both compact and higher-order accurate.

Recent years have seen growing popularity of compact schemes. This is primarily because of the two features that are possessed by compact schemes: higher accuracy and comparatively smaller stencils. A compact FD scheme only uses the grid points that are directly adjoining the node about which the differences are taken. This results in higher order of accuracy even in the case of smaller grid stencil. Furthermore, they can approximate and employ the gradients along with the function values at discrete nodes. Besides, the major advantage of compact schemes is that, in contrast to noncompact schemes, they always lead to a system of equations with a symmetric coefficient matrix having relatively smaller bandwidth. In some of the physical flow problems it is imperative to develop asymmetric FD approximations to tackle flow gradients. In the work of Hirsh [60] and Ciment *et al.* [20], the authors have introduced conditionally stable compact finite difference schemes to solve unsteady 2D CDE which are spatially fourth-order accurate and have second-order accuracy in time. In 1984, Gupta *et al.* [57] developed a compact FD method for steady CDE with variable coefficients. Later, in 1988, Noye and Tan [113] also reported a nine point implicit higher-order compact (HOC) scheme for 2D unsteady problem with constant coefficients. They successfully obtained a large region of stability of the scheme, which has a spatial accuracy of third-order and temporal accuracy of second-order. Significant advancement has been made in the last part of the previous century and early years of the current century in developing compact algorithms for N-S equations in particular, and convection-diffusion equations in general. In this regard, here we may refer a few contributions available in the literature [28, 33, 70, 76, 95, 96, 130, 148, 151, 179]. A detailed discussion on the historical development of compact schemes can be found in the work of Sen [130].

A traditional difficulty with all these methods mentioned above is their restricted application to regular uniform grids. With such meshes, it is challenging to resolve high gradient flow regions such as the shear layer. A nonuniform grid opens up the possibility of clustering grids in zones of large gradient and spreading out grid lines at other places. Furthermore, grids can be strongly stretched in the direction normal to the wall by clustering more grid points in the near-wall region. It is feasible to apply compact schemes developed on a uniform grid to nonuniform curvilinear grids by suitably defining coordinate transformation [115, 117, 118, 150, 181]. Even though such a procedure is more popular, it is fraught with major disadvantages. Transformation often leads to the appearance of cross-derivatives and is not an automatic choice for unsteady flows [61]. For nonsmoothly varying mesh spacing, transformation generates large errors. Further, a coordinate transformation leading to highly stretched meshes can have a destabilizing effect on overall discretization in general and convection term in particular as shown by Zhong [186]. Also, in the absence of explicit transformation, the added cost of the numerical grid generation [46, 86] is incurred. Thus, to maintain the accuracy and efficiency of numerical discretization, it is imperative to use a fully integrated approach where numerical schemes are developed by taking into account the stretching of the grid.

1.2 Motivation

In spite of significant development in numerical schemes, challenges still prevail concerning the applicability of compact schemes on nonuniform grids in particular. Thus, a window to explore the possibilities of developing compact schemes that can tackle flow problems on nonuniform grids remains wide open. Most of the compact schemes developed so far are efficient in solving fluid flow problems only, thereby ignoring the numerous physical systems involving heat transfer, which find significant importance and resemblance in various fields of science and engineering. Moreover, majority of the compact schemes that deal with nonuniform grids are based on the approach of transformation of the governing equation with the help of suitable conformal mapping. This approach comes with its inherent disadvantages that have been already mentioned in the previous section. Thus, there are scopes in establishing improved compact FD schemes that may work on both fluid flow and heat transfer problems on nonuniform meshes without resorting to transformation. Furthermore, there are problems in both 2D and 3D that possess steep boundary layers. These problems require very extensive computation and extremely clustered grids. We are also presented with the opportunity of developing a scheme that can solve these critical problems by exploiting the full potential of nonuniform grids. The motivation behind this work is to come up with a numerical scheme that can overcome these challenges and can be applied for problems with diverse complexities. We are particularly interested in generalizing the Padé based higher-order compact (HOC) scheme hitherto developed for uniform grids [130] to nonuniform grids and to investigate its order of convergence and applicability in diverse computational set-up.

1.3 Objective

The primary objectives of the thesis are as follows:

1. To develop a versatile compact Padé based finite difference scheme for steady

as well as transient convection-diffusion type equations that do not encourage domain transformation.

2. To investigate the adaptability of the scheme in both Cartesian and polar coordinate system.

3. To validate the algorithms thus developed for different test cases, including internal and external fluid flow problems on complex geometries.

4. To explore the natural and forced convection phenomena in different geometrical situations.

5. To attain physical insight into the fluid flow problems like driven cavity, flow past bluff bodies etc.

6. To accurately capture the transition period of the flow from steady to periodic state known as the Hopf bifurcation point.

7. To test both the spatial and temporal convergence of the developed schemes.

1.4 Organization of the work

The thesis has been organised into six chapters including the Introduction. Chapter 2 emphasizes on discretizing the CDE since it is going to serve as a prototype equation for the fluid and heat flow problems to be discussed. In this chapter, a new Padé based compact scheme is discerned on nonuniform grids for 3D generalized steady CDE. In Chapter 3, we further develop the compact scheme for transient CDE and propose a spatially and temporarily second-order accurate FD scheme. Further, the scheme is used to discretize unsteady N-S and Boussinesq equations. The scheme is employed to benchmark problems of fluid flow and heat transfer *viz.* lid-driven cavity, flow past square cylinder and natural convection in a square cavity. Later, the scheme is extended to the polar coordinate system in Chapter 4. Chapter 4 also includes the development of a novel third-order compact scheme. In Chapter 5, the scheme developed in the previous chapter is used to carry out an extensive study of flow past an impulsively started circular cylinder. In this chapter, the flow is simulated for Re ranging from 10 to 9500 and the results are extensively compared to those reported in various numerical and experimental studies. Finally, Chapter 6 summarizes and comments on the whole work and discusses the scope for future work.