Truncation Error Analysis for Diffusion Schemes in Boundary Regions of Unstructured Meshes

by

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF
MASTER OF APPLIED SCIENCE
in
The Faculty of Graduate and Postdoctoral Studies
(Mechanical Engineering)

THE UNIVERSITY OF BRITISH COLUMBIA
(Vancouver)
April 2015
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Abstract

Accuracy of numerical solution is of paramount importance for any CFD simulation. The error in satisfying the continuous partial differential equations by their discrete form results in truncation error and it has a direct influence on discretization errors. Discretization error, which is the difference in the numerical solution and the exact solution to a CFD problem, is generally the largest source of numerical errors. Understanding the relationship between the discretization and truncation error is crucial for reducing numerical errors. Studies have been carried out to understand the truncation-discretization error relationship in the interior regions of a computational domain but fewer for the boundary regions. The effect of different solution reconstruction methods, face gradient averaging schemes and boundary condition implementation methods on boundary truncation error in specific and overall truncation and solution error are the subject of research for this thesis. To achieve the goals laid out, the error has to be quantified first and then tests performed to compare the schemes. The Poisson’s equation is chosen as the model diffusion equation. The truncation error coefficients, analogous to the analytical coefficients of the spatial derivatives in Taylor series expansion of truncation error, are quantified using error metrics. The solution error calculation is made possible by a careful selection of exact solutions and their appropriate source terms for Poisson’s equation. Analytic tests are performed on a family of topologically regular meshes to test and verify the theoretical implementation of different schemes and to eliminate schemes performing poorly from consideration for numerical tests. The numerical tests are performed on unstructured triangular, mixed and pure quad meshes to extend the accuracy assessment for general meshes. The results obtained from both the tests are utilized to arrive at schemes where the overall truncation error and discretization error can be minimized simultaneously.
Preface

The research ideas and methods discussed in this thesis are the fruits of a close working relationship between Dr. Carl Ollivier-Gooch and Varun Prakash Puneria. The implementation of methods, the data analysis and the manuscript preparation were done by Varun Prakash Puneria with invaluable guidance from Carl Ollivier-Gooch throughout the process.
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Roman Symbols

\( \hat{n} \)  unit normal vector
\( e \)  edge vector
\( \mathcal{L} \)  continuous linear differential operator
\( f_B \)  continuous or discrete boundary condition function
\( A \)  Area
\( a \)  curved mesh aspect ratio
\( CV \)  control volume
\( EX, EY \)  gradient truncation error metric
\( E \)  flux integral truncation error metric
\( g \)  boundary gauss point
\( h \)  characteristic mesh length scale
\( k \)  mesh scaling factor
\( m \)  row number for analytic meshes
\( N \)  number of stencil members
\( R \)  residual, curved mesh radius ratio
\( s \)  length of control volume edges, mesh stretching factor
\( V \)  control volume area for integration
\( w \)  weights for least-squares method
\( x, y \)  Cartesian coordinates
List of Symbols

\( \mathbf{r} \) position vector

**Greek Symbols**

\( \alpha \) interior jump term coefficient

\( \alpha_B \) boundary jump term coefficient

\( \varepsilon \) discretization error

\( \lambda \) flux integral truncation error coefficients

\( \nu \) diffusion coefficient

\( \bar{\phi} \) control volume average of the variable

\( \Phi \) unknown variables vector

\( \phi \) solution variable, exact solution value

\( \rho \) random perturbations

\( \tau \) truncation error

\( \tilde{\phi} \) discrete form of the variable

\( \xi, \eta \) cell gradient truncation error coefficients

**Superscripts**

\( B \) boundary condition value

\( L \) left side

\( p, q \) polynomial exponent

\( R \) right side, reconstructed function

**Subscripts**

\( bdry \) boundary

\( F \) face

\( h \) discretized form of the continuous equation or variable

\( int \) interior
List of Symbols

\begin{itemize}
\item \textit{i} \hspace{1em} \text{reference control volume}
\item \textit{x,y} \hspace{1em} \text{Cartesian coordinates}
\item \textit{j} \hspace{1em} \text{neighboring control volume}
\end{itemize}
Acknowledgements

First and foremost, I would like to acknowledge my research supervisor, Dr. Carl Ollivier-Gooch, whose constant support, patience and guidance has been invaluable throughout the course of this research. Carl is a wonderful person and a great research adviser.

I am also grateful to my colleagues Alireza Jalali and Gary Yan at ANSLab research group for the suggestions and discussions which have been instrumental for my research. I would also like to thank David Zuniga from ANSLab research group for his invaluable time and the contributions to the mesh solver GRUMMP which made the test cases possible for the research.

Finally, my deepest appreciation is for my family, especially my mother “Durga” and father “Om”, and friends for their constant support and for their endless love and encouragement throughout my life.
Chapter 1

Introduction

Knowledge of fluid dynamics was not uncommon among the ancient civilizations. Design of arrows, spears, boats, irrigation systems, etc. demonstrate their knowledge in fluid flows. Notable contributions were made by Archimedes who formulated the laws of buoyancy and applied them to floating and submerged bodies. Leonardo da Vinci derived the equation of conservation of mass in one dimensional steady flow and his notes contained accurate descriptions of waves, jets, hydraulic pumps, eddy formation and both low and high drag designs. Sir Isaac Newton noted the effects of viscosity in diminishing the velocity of running water and his second law of motion was instrumental to the development of equations of fluid motion by Leonhard Euler. Euler’s idea to express the motion of fluids in partial differential equations was a major breakthrough, although it was limited in the sense that it did not account for the viscous forces.

The individual efforts of George Stokes and Claude Navier resulted in a complete set of governing equations for compressible viscous flows. However, the equations were too complicated to develop analytical solutions for arbitrary flows. This led to simplified forms of the equations with analytical solutions that applied to special cases of fluid flows, which were laminar or inviscid in nature. These special cases of flows had limited applications since most flows of engineering interests are viscous and turbulent.

The need for experiments has been indispensable to the advancement of understanding fluid dynamics. With limited analytical solutions, experimental fluid dynamics provided the much needed understanding of arbitrary fluid flows for complicated geometries. However, the costs that are necessary for both the experimental facility and the physical model to adequately simulate the prototype flow field restricts their application to modern day problems. Nevertheless, the data obtained from experiments is important for validating the mathematical solutions of the governing equations.

Up until twentieth century, theoretical and experimental fluid dynamics were the two approaches for the study of fluids. From the 1960s onward, the advent of computers and development of numerical algorithms has led to a third approach called Computational Fluid Dynamics (CFD). It has been an equal partner to the analytical and experimental approaches. Unlike experimental fluid dynamics, the
flow conditions and geometry of the problem can be easily varied to optimize the design process. Impractical situations like the re-entry of space vehicles can be simulated through CFD whereas analytical and experimental approaches are inadequate in present capacities.

The procedure of solving a fluid flow problem using CFD is broadly categorized into three parts [44, 41]: 1) Pre-processing which includes preparation of the computational domain and its discretization by meshing, 2) Numerical solver incorporates the mathematical expression of the governing laws along with initial and boundary conditions of the fluid flow problem to compute the numerical solution, and 3) Post-processing which is the analysis and visualization of the data generated from the solver. Figure 1.1 illustrates the schematic flow chart for procedures in CFD.

Figure 1.1: Flow chart for standard procedures in CFD
Chapter 1. Introduction

Pre-processing constitutes a major part of the efforts realized for any CFD project. The extraction of a computational domain after simplification of the physical geometry forms the first step for any CFD project. The computational domain should then be decomposed into smaller non-overlapping subdomains through the process of mesh generation. The accuracy of a numerical simulation is governed by the number of cells used to divide the domain. The larger the number of cells the better the resolution of the flow and the better the accuracy of the solution.

There are two types of mesh based on their topology, namely the structured and unstructured mesh types. In the structured mesh type, each of the grid element is identified by the indices \((i,j,k)\) which corresponds to their position in space. The regular connectivity of the mesh implicitly gives the address of the neighboring control volumes which makes it easier for performing calculations in the solver. The evaluation of fluxes, gradients and treatment of boundary conditions is greatly simplified by using structured grids. Structured grids commonly employ quadrilateral elements for two dimensions and hexahedral elements for three dimensions. Unstructured meshes lack the regular connectivity as observed in structured meshes. This means that the solver needs to process the mesh and determine the connectivity data with regards to the vertices, edges and neighboring cells. In two dimensions, the unstructured mesh is composed of triangular elements whereas for three dimensional meshes tetrahedral, prismatic and polyhedral elements can be used.

Compared to unstructured meshes, generation of structured meshes for simpler geometries is easier. The associated memory requirements, numerical error and computational time for structured meshes are less compared to unstructured meshes. However, for complex geometries, generating a structured mesh can be very time consuming or infeasible. Unstructured meshes offer the greatest flexibility in the treatment of complex geometries. The main advantage of unstructured meshes is the fact that the mesh generation can be performed automatically with minimal inputs, independent of the complexity of the domain. Unstructured meshes comprised of different element types are referred to as mixed grids whereas grids which have combined structured-unstructured grids are termed as hybrid grids. Figure 1.2 presents the different types of mesh that can be constructed around a 2D airfoil.

A popular method to accurately resolve the boundary layers for viscous flows is to use quadrilateral elements in two dimensions and prismatic or hexahedral elements in three dimensions near the solid walls [4]. Usually, viscous flow regions require high aspect ratio grid cells and the ways to achieving this condition is by generating 90 degree triangles or rectangles in shear layers [7, 38, 42]. In three dimensions, this can be achieved by using prismatic or hexahedral cells near the boundary.
Chapter 1. Introduction

(a) Structured

(b) Unstructured

(c) Mixed

Figure 1.2: Description of mesh types
Chapter 1. Introduction

The development of flow simulation software begins with the mathematical modeling of physical phenomena. It is here that the decision to omit or consider different aspects of the flow to be modeled are made. The extent to which the physical phenomena is modeled will determine the extent to which the numerical simulation will represent the actual flow scenarios. For instance, whether the flow is compressible or incompressible, inviscid or viscous, laminar or turbulent will determine the set of mathematical equations, typically partial differential equations (PDEs), to be solved. Even if we chose to solve the flow of certain nature, say incompressible turbulent flows, the extent to which the flow features need to be resolved will determine the type of turbulence models needed. For example, the Spalart-Allmaras [39] turbulence model is a good RANS model for aerodynamic flows but computer intensive models like Large Eddy Simulation (LES) or Direct Numerical Simulation (DNS) are essential for complex or separated turbulent flows. The requirements to model the physical phenomena are not limited to turbulence but may also include multiphase interactions, chemical reactions and electromagnetic phenomena. The tremendous requirements on computational resources to solve complex phenomena like turbulence or chemical reactions necessitates approximation by physical modeling and the errors associated with it. The study of these errors, called physical modeling errors, is not within the scope of this research.

The initial values of flow variables must be specified at all solution points in the domain. The initial conditions determine the state of the fluid at time $t = 0$ or at the first step of an iterative scheme. A good initial guess implies that convergence to a steady-state solution will be faster. Boundary conditions along with the computational domain give the information on the physical problem that is being solved for. For instance, if the computational domain is that of an airfoil with an appropriate mesh, the boundary conditions will dictate if we are solving a subsonic or a supersonic flow. Some of the common boundary conditions are the wall, inlet and outlet, symmetry, periodic, etc. Many common boundary conditions are classified as Dirichlet or Neumann boundary conditions. If the variable is specified along the boundary, it is known as the Dirichlet type whereas if the normal gradient of the variable is specified, it is called the Neumann type boundary condition. A linear combination of the Dirichlet and Neumann types can also be specified and is known as the Robin type boundary condition.

After the governing equations are chosen and initial and boundary conditions are set, the PDEs need to be discretized so that they can be solved on a computer. There are three popular methods of discretization for the PDEs: finite difference methods, finite element methods and finite volume methods.

The finite difference method was the first method applied to calculate numerical solution of differential equations. The solution variables $\Phi$ are stored as point
values at the grid points. Using Taylor series expansions, the derivatives of the variables $\Phi$ are approximated by their finite difference equations in terms of their point wise solution values. These finite difference approximations are substituted for the derivatives of the variables $\Phi$ in the governing equations at every grid point, resulting in a set of algebraic equations in terms of point wise solution variables at the grid points. Solving these algebraic expressions for the entire domain gives us the solution data. The finite difference method is very simple, effective and easy to obtain higher order schemes on regular grids. However, the conservation of mass, momentum and energy is not enforced unless special care is taken and this approach is impractical for unstructured grids.

The finite element method was initially developed for structural stress analysis and is also applied for fluid dynamics. This method uses simple piecewise basis functions, which are valid on elements and describe the local variations of the unknown variables $\Phi$. The choice of basis functions determines the accuracy of the scheme. This solution approximation is substituted into the governing equations; and since it does not satisfy the equations exactly, a residual is obtained. The residuals are minimized in some sense by multiplying them with weighing functions and integrating. The resulting set of algebraic equations are solved for the unknown coefficients of the approximating function. This method is easily extendable to unstructured meshes and higher order schemes. However, the conservation of mass, momentum and energy, though possible, is not trivial in flows with discontinuities.

The finite volume method uses integration of the governing equations of fluid flow over each control volume of the domain. Applying Gauss’s theorem leads to an equation relating the amount of a conserved quantity in a control volume to the flux of that quantity through the control volume boundary. The fluxes, in turn, are approximated in terms of control volume averages, which results in a system of algebraic equations. The solution field is obtained by solving this system of equations. It is the easiest method to understand and the approximated terms have physical meanings which makes it a popular method of discretization for CFD. Mass, momentum and energy are directly conserved using this method and it can be easily implemented on structured and unstructured grids.

Irrespective of the type of discretization used, the approximation leads to an error due to the difference in the discrete and continuous equations called the truncation error. The error in satisfying the exact solution to the continuous PDEs by the solution to the discretized equations is called the discretization error. Discretization error is the largest source of numerical errors (others being round-off error, iterative convergence error, etc). Truncation error acts as a local source for the transport of discretization error [35] and it is usually estimated by replacing all the nodal values in the discrete approximation by a Taylor series expansion about a
1.1. Motivation

The convergence of truncation errors is generally a good indicator of convergence of discretization errors on structured meshes; however, the degradation of convergence for truncation errors doesn’t necessarily imply a degradation in discretization errors for unstructured meshes. Nevertheless, many methods use the truncation error for mesh adaptation to reduce the discretization errors [35, 46]. By reducing the truncation errors, it is possible to reduce the discretization errors.

The finite volume method of discretization is used for the research presented in this thesis. A good CFD solver incorporates discretization techniques suitable for the treatment of the key physical phenomena, convection and diffusion, as well as any source terms associated to give a convergent, consistent and stable solution. The underlying physical phenomena is usually complex and non-linear, hence the solver should have a stable time marching or iterative scheme for computing the solution. The CFD solver code ANSLib [33] developed by the Advanced Numerical Simulations Laboratory (ANSLab) has all the characteristics of being a good solver and is chosen for the numerical experiments conducted in this research. It uses an edge based formulation to handle mixed grids with a robust numerical scheme. ANSLib allows the users to specify physics of their problem by providing code snippets to compute interior and boundary fluxes, source terms, initial conditions and by specifying constraints on the solution at the boundaries.

The final stage of CFD is post-processing. The visualization of vector plots, domain geometry, 2D and 3D surface plots, solution and error contours come under post-processing. There are many tools available in the market for post-processing. We have chiefly employed Paraview and MATLAB for post-processing along with common plotting tools.

1.1 Motivation

The numerical simulation of fluid flows is affected by three forms of errors, namely: the geometry modeling, physical modeling and numerical errors. Geometry modeling errors are related to the transformation from the physical domain to a computational domain by either omitting or simplification of complex parts of the geometry. They are usually unavoidable and can help allocate resources to capture important features of the flow. Omitting rivets in the structures or modification of a pointed trailing edge are examples of geometry modeling.

Physical modeling errors pertain to the effective modeling of physical phenomena, for instance turbulence or real gas effects, by mathematical models. Often modeling is required for turbulence, boundary conditions, multi-phase models, etc. The inadequacy in predicting the physical phenomena accurately by such models...
leads to physical modeling errors. Both geometry and physical modeling errors are outside the scope of this thesis, which focuses on numerical errors.

Current experiments have shown that the numerical errors are as large as the physical modeling errors and it is significantly important to reduce them. The first three AIAA Drag Prediction Workshops (DPW) [23, 21, 26] used similar wing geometries to compare the computational data with the experimental data. The first two workshops used a DLR-F4 and DLR-F6 wing geometry respectively and the results revealed significant scatter in terms of drag prediction and agreement with the experimental data. The scatter was attributed to regions of turbulent separated flow in the test cases and a wing body fairing was designed and added to the DLR-F6 wing body configuration in the third DPW workshop, so as to suppress flow separation in the wing-body juncture. The results for the third workshop and the overview of the three workshops [28] revealed that the scatter was not just a result of physical modeling errors but also numerical errors. The first three workshops also established that the use of different solvers, turbulence models, grid types or grid constructions all contribute to the variation in the results.

The fifth AIAA Drag Prediction Workshop [24] focused on reducing grid-related errors by performing a grid refinement study on a common grid sequence derived from a multiblock structured grid. The study had six different levels of grid refinement ranging from $0.64 \times 10^6$ cells to $136 \times 10^6$ cells, with structured overset and hexahedral, prismatic, tetrahedral and hybrid unstructured grid formats tested with different turbulence models. The study concluded that there was no clear break-outs with regards to grid type or turbulence model with discretization errors and turbulence modeling still being the significant contributors to the scatter in results. Overall, different grid types, grid constructions, and discretization schemes had different results even when the solution was converged.

Discretization errors, which are a major source of numerical errors, are often most difficult to calculate for general flows. Discretization error arises out of the interplay between the chosen discretization scheme, the mesh quality (cell size, shape, anisotropy, etc.), the mesh resolution and the solution and its derivatives. Roy [36] has discussed the issues related to discretization error estimators and has emphasized that for any method to give a reliable estimate, it is necessary to achieve the asymptotic range of solution convergence. As difficult as it is to estimate discretization error, we utilize the understanding that it is transported through the domain in much the same fashion as the solution in the underlying mathematical model [14, 35] and is locally generated according to the truncation error. Roy [36] showed that for a linear differential operator $\mathcal{L}$, the truncation error $\tau$ can be used to estimate the discretization error $\varepsilon$, as

$$\mathcal{L}(\varepsilon) = -\tau$$

(1.1)
1.1. Motivation

Figure 1.3: One dimensional grid for convection-diffusion equation

known as the error transport equation. Banks et al. [1] extended the error transport method to estimate discretization error for finite volume discretizations of nonlinear hyperbolic equations and demonstrated the approach to provide useful error estimates. The scope of this research is limited to linear problems, however. Equation 1.1 shows that the discretization error evolves the same way as the solution does, with the truncation error being the driving source. For some cases, the careful refinement of the mesh in regions of high truncation error can lead to a reduction in discretization error as shown in [46]. Mesh adaptation based on truncation error is observed to give the lowest discretization errors [46, 35] and motivates us to understand the relation between the two types of errors.

In this thesis, we concern ourselves with a general approach to reduce truncation error irrespective of the solution type and do not attempt at either estimation of truncation error or mesh adaptation. Consider a one dimensional convection-diffusion equation discretized using the finite volume approach on a one dimensional grid [17]. Most flows fall into the category of convection and diffusion and hence it serves as an ideal model to explain the idea behind our approach.

\[ \mathcal{L}(\phi) = \frac{\partial \phi}{\partial x} - \nu \frac{\partial^2 \phi}{\partial x^2} = 0 \]  

A finite volume discretization of the equations requires the averaging over the control volume \( i \). The advection term when averaged over the control volume takes the form,

\[ \overline{\frac{\partial \phi}{\partial x}} = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left( \frac{\partial \phi}{\partial x} \right) dx = \frac{\phi_{i+\frac{1}{2}} - \phi_{i-\frac{1}{2}}}{\Delta x} \]  

The solution values are stored at the nodes for the uniform mesh shown in the Figure 1.3. To calculate the averaged gradient in the Equation 1.3, one would need the values of the solution variable on the control volume boundaries. For a general
1.1. Motivation

unstructured mesh, we would need solution reconstruction to better approximate the required data. However, for purposes of illustration here, we use a first order upwind approximation to estimate the solution variables at the control volume boundaries. Thus we have,

\[ \phi_{i+\frac{1}{2}} \approx \bar{\phi}_i, \ \phi_{i-\frac{1}{2}} \approx \bar{\phi}_{i-1} \]  

(1.4)

and the averaged gradient would be

\[ \frac{\partial \phi}{\partial x} = \frac{\bar{\phi}_i - \bar{\phi}_{i-1}}{\Delta x} \]  

(1.5)

To determine the accuracy of the scheme, we use Taylor series expansion to calculate the control volume averages in terms of the solution and derivatives at the reference point of control volume \(i\).

\[ \bar{\phi}_i = \frac{1}{\Delta x} \int_{x_i-\frac{1}{2}}^{x_i+\frac{1}{2}} \left( \phi_i + \frac{\partial \phi}{\partial x} \bigg|_{x_i} (x-x_i) + \frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_{x_i} (x-x_i)^2 + \frac{1}{6} \frac{\partial^3 \phi}{\partial x^3} \bigg|_{x_i} (x-x_i)^3 \ldots \right) \]

\[ = \phi_i + \frac{1}{24} \frac{\partial^2 \phi}{\partial x^2} \bigg|_{x_i} (\Delta x)^2 + O(\Delta x)^4 \]  

(1.6)

\[ \bar{\phi}_{i-1} = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left( \phi_i + \frac{\partial \phi}{\partial x} \bigg|_{x_i} (x-x_i) + \frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_{x_i} (x-x_i)^2 + \frac{1}{6} \frac{\partial^3 \phi}{\partial x^3} \bigg|_{x_i} (x-x_i)^3 \ldots \right) \]

\[ = \phi_i - \frac{\partial \phi}{\partial x} \bigg|_{x_i} (\Delta x) + \frac{13}{24} \frac{\partial^2 \phi}{\partial x^2} \bigg|_{x_i} (\Delta x)^2 - \frac{5}{24} \frac{\partial^3 \phi}{\partial x^3} \bigg|_{x_i} (\Delta x)^3 + O(\Delta x)^4 \]  

(1.7)

Substituting the above expansions into the Equation 1.5, the resultant gradient turns out to be first order accurate with a leading error term of \(-\frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_{x_i} (\Delta x)\) which is the truncation error for the gradient approximation.

\[ \frac{\partial \phi}{\partial x} = \frac{\partial \phi}{\partial x} \bigg|_{x_i} + \frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_{x_i} (\Delta x) + \frac{5}{24} \frac{\partial^3 \phi}{\partial x^3} \bigg|_{x_i} (\Delta x)^2 + O(\Delta x)^3 \]  

(1.8)

Applying a similar procedure for the diffusion term in Equation 1.2, the centered difference results in a second order accurate approximation:

\[ \frac{\partial^2 \phi}{\partial x^2} = \frac{\partial^2 \phi}{\partial x^2} \bigg|_{x_i} + \frac{1}{8} \frac{\partial^4 \phi}{\partial x^4} \bigg|_{x_i} (\Delta x)^2 + O(\Delta x)^4 \]  

(1.9)
The discrete approximation to the convection-diffusion equation can finally be written as:

\[
\mathcal{L}_h(\phi) = \frac{\partial \phi}{\partial x} - v \frac{\partial^2 \phi}{\partial x^2} = \left( \frac{\partial \phi}{\partial x} \bigg|_i - v \frac{\partial^2 \phi}{\partial x^2} \bigg|_i \right) - \frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} (\Delta x) + (1.10)
\]

\[
\frac{5}{24} \frac{\partial^3 \phi}{\partial x^3} \bigg|_i (\Delta x)^2 - \frac{v}{8} \frac{\partial^4 \phi}{\partial x^4} \bigg|_i (\Delta x)^2 + \ldots
\]

The operator \( \mathcal{L}_h \) is the discrete operator whereas on the right hand side, we can identify the continuous PDE for convection-diffusion. The entire equation can be re-written in the form derived in the works of Roy [35] as shown in the Equation 1.11. A careful substitution of the discrete and exact solutions to the PDE will lead us to the derivation shown in the Equation 1.1

\[
\tau(\phi) = \mathcal{L}_h(\phi) - \mathcal{L}(\phi)
\]

The truncation error in Equation 1.10 highlights that the discretization is formally first order and that the leading error term adds extra diffusion into the system. The even order derivatives have a tendency to smear the sharp gradients of the solution and are said to be diffusive in nature whereas odd order derivatives induce an oscillatory behavior in the smooth regions of the solution and are said to be dispersive in nature.

Truncation error is dependent on the derivatives of the solution and their associated coefficients. Schemes which are independent of the solution derivatives but effective in reducing the truncation error coefficients will in general reduce truncation error and in turn discretization error. Previous work has shown that the truncation error coefficients are influenced by the selection of reconstruction methods, face gradient averaging schemes, jump terms, etc. [17, 30, 45] in the numerical schemes. This observation lays the foundation for this thesis where the goal is to analyze the effects of different discretization schemes and boundary condition implementations in bringing out the desired results in solution accuracy.

Jalali and Ollivier-Gooch [18, 19] have performed analytical and numerical experiments on cell-centered finite volume discretizations of diffusion and convection equations. Their analysis involved the computation of the coefficients of Taylor series expansion for the truncation error and have demonstrated the methods to quantify both the truncation and discretization errors. Yan et al. [45] performed truncation and discretization error analysis for diffusion problems based on vertex-centered discretization. In solving Poisson’s equation using the finite volume approach, Diskin et al. [10] compared cell-centered and vertex-centered schemes and
concluded that there is little difference in the accuracy of the two approaches at an equivalent number of degrees of freedom.

The previous works on diffusion and convection were restricted to the interior domain of the mesh and the influence of discretization schemes on the boundary control volumes is largely unclear. Moreover, it is not known which implementations of the boundary conditions are more accurate. The effect of different solution reconstruction methods, face gradient calculations, boundary condition implementation methods and modifications to meshes on the boundary truncation error and overall discretization error needs to be studied. Given that the discretization error and truncation error are related to each other, the understanding of the relationship between the two errors is not very clear, either.

Thus, our primary objective for this research is to explore the ways in which truncation error in the boundary regions of a mesh can be reduced while the overall goal is to reduce both the truncation and discretization errors globally. A detailed objective of this thesis is presented in the next section.

1.2 Objectives

In this thesis, we define our problem statement as the truncation error analysis for diffusion schemes in the boundary regions of unstructured meshes and attempt to reduce interior and boundary truncation error as well as the solution error. Poisson’s equation is used as the model diffusion equation and vertex-centered control volumes are defined for the finite volume discretization. We study the influence of different discretization schemes and boundary condition implementation methods on truncation and discretization error and also try to decipher the relationship between the truncation error and the solution accuracy. The scope of this research is limited to isotropic and stretched 2-D meshes, both triangular and mixed.

Among the type of discretization schemes, we chiefly inspect the differences in the use of popular solution reconstruction methods which are the least-squares and Green-Gauss methods. Green-Gauss method has been traditionally popular for viscous flows [9, 13, 27]. It has also been noted to suffer from decoupling issues when quadrilateral meshes are used. Thomas et al. [40] and Diskin and Thomas [9] have shown remedies to counter this issue associated with Green-Gauss method. The least-squares method is one of the preferred methods for solution reconstruction in the literature [8, 31, 20, 25] and was found to be comparable or even better than the Green-Gauss method for accurate gradient calculation. It paves the way for higher order reconstruction whereas the Green-Gauss method is restricted to second order. Apart from gradient calculation at the center of control volumes, the calculation of face gradients on control volume boundaries influence
1.2. Objectives

The use of ghost cells as a method of boundary condition implementation is well known and a brief description of the method can be found in Blazek [4] and Leveque [22]. Cary et al. [6] used ghost cells for boundary condition implementation in Boeing’s BCFD solver in a cell-centered approach and found an improved drag prediction for a NACA 0012 airfoil section using Euler’s equations. However, the impact of ghost cells in reducing the truncation error is unknown and we study this boundary condition implementation on vertex-centered approach with a second order reconstruction in the ghost cells.

An alternate method of applying the boundary condition is to use the boundary condition information for solution reconstruction in the boundary control volumes and thereby calculating the flux at the boundary edges. This approach is presented in the works of Ollivier-Gooch and Van Altena [34], where the boundary conditions at the Gauss points for flux integration are used as hard constraints, which along with information from neighboring control volumes, is used to reconstruct gradients in a least-squares sense. This approach and its variants are explored to devise schemes efficient in reducing truncation error and improve solution accuracy.

Finally, the use of jump terms [30] to introduce a damping term based on the jump in solution values at control volume interfaces has been proven to give accurate solution for diffusion problems. Jalali [17] and Yan et al. [45] have found jump terms to be effective in modifying truncation error coefficients for interior control volumes. The current research explores the potential of this method to devise new boundary treatment methods and its impact on boundary truncation error as well.

The evaluation of different discretization schemes and boundary treatment methods is conducted in two stages. In the first stage, a qualitative and quantitative comparison is performed analytically for different test cases for meshes which are general in nature. These tests are performed to ascertain the asymptotic behavior of the schemes developed. They also present a platform to verify the schemes on a variety of systematically perturbed meshes so that the implementation can be corrected, compared and schemes performing below expectations be eliminated.

In the second stage, the numerical experiments are performed with schemes filtered from analytical tests to re-affirm the observations found in analytical results. The numerical tests provide a robust testing mechanism where the schemes are tested with different boundary conditions, solution types and meshes to assess the applications and limitations of schemes developed. Isotropic and stretched mesh sequences are generated for pure triangular and mixed meshes along with isotropic pure quadrilateral meshes. Each sequence has four systematically refined meshes to study the asymptotic convergence of schemes as well.

Thus, results for a variety of different treatments to the boundary cells, solution reconstruction and boundary stencil are presented in this work with emphasis laid
1.3 Outline

Chapter 2 lays the theoretical foundation for the research presented in this thesis. An overview of the finite volume method used for solving the diffusion equation by constructing vertex-centered control volumes is given in this chapter. The key aspects of the solver which include solution reconstruction, face gradient calculation and flux integration, are discussed in detail. The differences in the interior and boundary control volumes are highlighted with respect to the reconstruction stencils and other relevant factors. The chapter discusses in detail the schemes developed or considered to test for reducing the truncation errors which include modification to the stencil, use of boundary constraints and the use of jump terms.

The methodologies for the calculation of truncation error, both analytically and numerically, are presented in Chapter 3. The Method of Manufactured Solutions is also discussed for the calculation of discretization error.

Chapter 4 presents the analytical and numerical results for pure triangular meshes. The analytic section presents the challenges faced in the implementation of the methods and the remedies applied to standard methods for obtaining better results. The schemes performing better in the analytic section are taken forward for the implementation in the numerical solver. Chapter 5 presents the analytical and numerical results for the mixed and pure quadrilateral meshes and the challenges with the implementation for mixed meshes are highlighted in the analytic and numerical sections. The results for analytic and numerical sections are compared and contrasted with the results for triangular meshes. The differences and similarities in isotropic and stretched boundary layered meshes are also presented in both the chapters. Overall, the schemes performing best for reducing the truncation and discretization errors are explored to seek guidelines for achieving simultaneous reduction in different forms of errors for all the types of mesh tested in this thesis.

The summary of approaches taken in this thesis are presented in the Chapter 6 along with concluding remarks drawn from the results. The scope for future work is also laid out in this chapter.
Chapter 2

Background

A background of the CFD practices used in the current research is presented in detail in this chapter. First a brief overview of the relevant aspects of CFD for solving a diffusion problem using the finite volume discretization is given. The formulation for solution reconstruction using methods like least-squares and Green-Gauss are explained. Next, numerical flux calculation and rules for flux integration are given. Finally, the rationale and methodology for different boundary treatment methods experimented with in this thesis are presented.

2.1 Finite Volume Approach

The finite volume method is a robust method for solving fluid flow problems as it directly utilizes the conservation laws of fluids. The first step of the finite volume approach is to divide the physical domain into arbitrary polyhedral (3D) or polygonal (2D) grid elements and then to discretize the integral form of the governing equations over each control volume. There are two basic approaches to defining the control volumes with respect to the grid. They are the (i) cell-centered approach and (ii) vertex-centered approach. In cell-centered approach, the control volumes are identical to the primal grid cells and the solution values are stored at the centroids of the primal cells. On the other hand in vertex-centered approach, the solution values are stored at the vertices and the control volumes are the mesh dual. In our current research we limit ourselves to two dimensions although the extension to three dimensions for the schemes presented in this thesis is pretty straightforward. We use the vertex-centered approach with vertices as the reference points and the control volumes defined by the median dual. The median dual is constructed by connecting the mid points of the faces and the centroids of the primal cells sharing the reference vertex. Figure 2.1 gives an illustration of the different approaches discussed here.

In current research, the Poisson equation, $\nabla^2 \phi = S$, is used as a model equation for diffusion. The differential form of Poisson’s equation is integrated over the control volume and the application of the divergence theorem gives us the finite volume formulation for Poisson’s equation, taking the form as shown:
2.2. Solution Reconstruction

Figure 2.1: Control volume illustration

\[ \oint_{\partial V} \nabla \phi \cdot \hat{n} \, ds = \int_{V} S \, dA \]  \hspace{1cm} (2.1)

where \( \hat{n} \) is the outward normal vector and \( ds \) is the infinitesimal for the integration along the edges of the control volume. The solution for the Poisson’s equation is a steady state solution where the left hand side of Equation 2.1 is the flux integral along the perimeter of the control volume. The elliptic nature of Poisson’s equation implies that the solution in the interior is strongly affected by the boundary conditions.

2.2 Solution Reconstruction

The simplest method of reconstruction is to assume a constant solution value in the control volumes, which is basically a first order reconstruction. However, the scheme is too diffusive and leads to excessive growth of shear layers [4]. Thus, a second or higher order reconstruction is needed. The Green-Gauss method is popularly employed for second order accurate flux calculations in the literature [9, 13, 27, 15]. Higher order accurate methods first appeared in literature as early as the 1990s, when Barth and Fredrickson [3] presented a method for k-exact reconstruction and use of Gaussian quadrature rules for high order flux evaluations. The works of Ollivier-Gooch and Van Altena [34] detail the inclusion of mean and boundary constraints in the framework of developing higher order schemes for the advection-diffusion equation.
2.2. Solution Reconstruction

The evaluation of solution and gradients to the desired level of accuracy is necessary for accurate flux integration and ultimately a steady solution to the Poisson’s equation. The following sections discuss the traditionally popular Green-Gauss and least-squares methods to obtain a second order accurate solution reconstruction. The Green-Gauss method presented in this work assumes a constant gradient in the primal grid cells and the gradient calculation takes an algebraically simpler form for triangular mesh.

Next, the framework for the least-squares method is presented where the conditions to be satisfied for a consistent solution reconstruction of desired accuracy are laid out. This is followed by the weighted second order least-squares formulation where the unknown derivatives of solution variables are evaluated followed by the advantages of the least-squares method over the Green-Gauss method. At the end of this section we also highlight the subtle differences in the reconstruction stencils for interior and boundary control volumes which we anticipate to affect the accuracy of gradient calculation and in turn truncation and discretization errors.

2.2.1 Green-Gauss Method

The gradients required for numerical flux evaluation are directly calculated using the Green-Gauss method. The gradients are calculated using the Green-Gauss formula [11, 43, 15] over the primal cells even though the FVM formulation is vertex based. Let us consider a mixed element grid as shown in the Figure 2.2. For fully triangular grids, the formulation is equivalent to a Galerkin finite element scheme with a linear basis function [2]. The Green-Gauss formula is

\[
\int_V \nabla \phi dA = \oint_{\partial V} \hat{\phi} \hat{n} ds \tag{2.2}
\]

The gradients at the dual face BC contained in the triangular cell is calculated as

\[
\nabla \phi_{BC} = \nabla \phi_{021} = \frac{1}{2A_{021}} \left[ \begin{array}{c}
(\bar{\phi}_0 + \bar{\phi}_2)(y_0 - y_2) + (\bar{\phi}_2 + \bar{\phi}_1)(y_2 - y_1) + (\bar{\phi}_1 + \bar{\phi}_0)(y_1 - y_0) \\
-(\bar{\phi}_0 + \bar{\phi}_2)(x_0 - x_2) - (\bar{\phi}_2 + \bar{\phi}_1)(x_2 - x_1) - (\bar{\phi}_1 + \bar{\phi}_0)(x_1 - x_0)
\end{array} \right] 
\tag{2.3}
\]

where \( \nabla \phi_{021} \) is the gradient evaluated on the primal cell identified by the subscripts. For the dual face AB contained in the quad cell, the gradient is evaluated using a combination of the Green-Gauss formula and an edge derivative correction to avoid decoupling and give improved gradients [4, 11].

\[
\nabla \phi_{AB} = \nabla \phi_{0432} + \left[ \frac{\bar{\phi}_2 - \bar{\phi}_0}{r_2 - r_0} - \nabla \phi_{0432} \cdot e_{02} \right] e_{02} \tag{2.4}
\]
2.2. Solution Reconstruction

Figure 2.2: Gradient reconstruction for mixed cell interface using Green-Gauss method

\( \mathbf{r}_i \) is the position vector for the node \( i \) whereas \( \mathbf{e}_{02} \) is the unit vector in the direction of the edge \([0,2]\) given by

\[
\mathbf{e}_{02} = \frac{\mathbf{r}_2 - \mathbf{r}_0}{|\mathbf{r}_2 - \mathbf{r}_0|}
\]  

(2.5)

Note that for both the dual faces AB and BC, the edge derivative is recovered. Mathematically, this means

\[
\nabla \phi_{BC} \cdot \mathbf{e}_{02} = \nabla \phi_{AB} \cdot \mathbf{e}_{02} = \frac{\phi_2 - \phi_0}{|\mathbf{r}_2 - \mathbf{r}_0|}
\]

(2.6)

The above gradient calculation is found to be make the Green-Gauss gradients less susceptible to the odd-even decoupling [16]. The scheme presented in this section has been shown by Thomas et al. [40] and Diskin and Thomas [9] to possess second order accuracy for general isotropic mixed meshes with regards to discretization error.

Our experiments revealed that the truncation error was more sensitive to the fact that the vertex doesn’t coincide with centroid of the control volume. This discrepancy is observed to give \( O(h^{-1}) \) order for truncation error where \( h \) is the characteristic mesh size and was remedied by using centroid locations instead of node locations for the gradient calculation.

2.2.2 Least-Squares Method

The first step in using the least-squares method is to formulate the conditions necessary for a consistent reconstruction scheme. The reconstruction design crite-
2.2. Solution Reconstruction

ria [3, 32] requires the method to conserve the mean of control volumes, have a compact support and exactly reconstruct polynomials of required degree. The framework for least-squares is built in the following sub-section by satisfying the reconstruction design criteria followed by the second order weighted formulation to obtain the unknown derivatives.

2.2.2.1 Framework for Least-Squares Method

Higher order accurate reconstruction and an equally accurate flux integration method are essential for an accurate finite volume scheme. In this sub-section, we limit the discussion to the development of a general reconstruction framework to obtain the desired level of accuracy. Our goal is to first express the solution as a continuous Taylor series polynomial about the reference point $(x_i, y_i)$

$$
\phi^R_i(x, y) = \phi_{i} + \frac{\partial \phi}{\partial x} \bigg|_i (x - x_i) + \frac{\partial \phi}{\partial y} \bigg|_i (y - y_i) + \\
\frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_i (x - x_i)^2 + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_i (x - x_i)(y - y_i) + \\
\frac{1}{2} \frac{\partial^2 \phi}{\partial y^2} \bigg|_i (y - y_i)^2 + \ldots
$$

In Equation 2.7, the solution $\phi^R_i$ is the reconstructed solution at any point $(x, y)$ about the reference control volume $i$ provided we know the solution values and the derivatives $\frac{\partial^{1+\ell} \phi}{\partial x^{\ell} \partial y^{\ell}}$ at that point. The derivatives and the solution values are the coefficients of the Taylor polynomial and the degree of this polynomial determines the order of reconstruction. Second order accuracy for instance can be obtained if we know the gradients in $x$ and $y$, as can be seen in Equation 2.8. Such a reconstruction is linearly varying in the control volume. The implications can be seen in a cell-centered scheme where the pointwise solution value at the centroid naturally represents the control volume average at second order accuracy. In a vertex-centered approach however, the control volume average differs from the pointwise solution value at the vertex with a first order error:

$$
\phi^R_i(x, y) = \phi_{i} + \frac{\partial \phi}{\partial x} \bigg|_i (x - x_i) + \frac{\partial \phi}{\partial y} \bigg|_i (y - y_i) + O(\delta x^2, \delta y^2)
$$

The coefficients of the Taylor polynomial are chosen such that the error in satisfying the mean solution value in the stencil control volumes is minimized. Enforcement of the mean in the reference control volume requires that
2.2. Solution Reconstruction

\[ \bar{\phi}_i = \frac{1}{A_i} \int_{V_i} \phi^R(x,y) dA \] (2.9)

Substituting Equation 2.7 in the mean constraint requirement, one can see that,

\[ \bar{\phi}_i = \frac{1}{A_i} \int_{V_i} \phi^R(x,y) dA = \phi_i + \frac{\partial \phi}{\partial x} \bigg|_i x_i + \frac{\partial \phi}{\partial y} \bigg|_i y_i + \frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_i x_i^2 + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_i x_i y_i + \frac{1}{2} \frac{\partial^2 \phi}{\partial y^2} \bigg|_i y_i^2 + \ldots \] (2.10)

where the geometric moments for the reference control volumes are defined as

\[ \bar{x}^p y^q_i = \frac{1}{A_i} \int_{V_i} (x - x_i)^p (y - y_i)^q dA \] (2.11)

By observation, the above integral can be easily calculated by using Green's theorem to convert into a line integral along the boundary of control volume. The integration can now be evaluated using Gaussian quadrature rules for desired accuracy

\[ \bar{x}^p y^q_i = \frac{1}{A_i(p+1)} \int_{\partial V_i} (x - x_i)^p (y - y_i)^q dy \] (2.12)

For \( k \) exact reconstruction, the Taylor series expansion of \( \phi_i^R \) must be carried out through until the \( k^{th} \) derivatives. The derivatives are computed by seeking to minimize the error in predicting the mean value of the solution for control volumes in the stencil \( \{V_j\}_i \). The mean value for neighboring control volumes is calculated as

\[ \frac{1}{A_j} \int_{V_j} \phi^R(x,y) dA = \phi_j + \frac{\partial \phi}{\partial x} \bigg|_j x_j + \frac{\partial \phi}{\partial y} \bigg|_j y_j + \frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_j x_j^2 + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_j x_j y_j + \frac{1}{2} \frac{\partial^2 \phi}{\partial y^2} \bigg|_j y_j^2 + \ldots \] (2.13)

The calculation of moments for every neighboring control volume in the stencil \( \{V_j\}_i \) about reference control volume is simplified by replacing \( (x - x_i) \) and \( (y - y_i) \) with geometric moments.
2.2. Solution Reconstruction

\( y_i \) with \( (x - x_j) + (x_j - x_i) \) and \( (y - y_j) + (y_j - y_i) \) respectively. Expanding and integrating Equation 2.13

\[
\frac{1}{A_j} \int_{\hat{V}_j} \phi_i^p(x, y) dA = \phi_i + \frac{\partial \phi}{\partial x} \bigg|_i (\bar{x}_j + (x_j - x_i)) + \frac{\partial \phi}{\partial y} \bigg|_i (\bar{y}_j + (y_j - y_i)) + \quad (2.14)
\]

\[
\frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_i (x^2_{ij} + 2\bar{x}_j(x_j - x_i) + (x_j - x_i)^2) + \\
\frac{\partial^2 \phi}{\partial x \partial y} \bigg|_i (\bar{x}_y + \bar{x}_j(y_j - y_i) + \bar{y}_j(x_j - x_i) + (x_j - x_i)(y_j - y_i)) + \\
\frac{1}{2} \frac{\partial^2 \phi}{\partial y^2} \bigg|_i (y^2_{ij} + 2\bar{y}_j(y_j - y_i) + (y_j - y_i)^2) + ...
\]

The geometric terms from the Equation 2.14 can be written in a general form as

\[
\hat{x}^p\hat{y}^q_{ij} = \frac{1}{A_j} \int_{\hat{V}_j} ((x - x_j) + (x_j - x_i))^p((y - y_j) + (y_j - y_i))^q dA \quad (2.15)
\]

\[
= \sum_{l=0}^{q} \sum_{k=0}^{p} \binom{p}{k} \binom{q}{l} (x_j - x_i)^k(y_j - y_i)^l \hat{x}^{p-k} \hat{y}^{q-l}_{ij}
\]

Using the hat notation for the geometric terms, Equation 2.14 is re-written as

\[
\hat{\phi}_j = \phi_i + \frac{\partial \phi}{\partial x} \bigg|_i \hat{x}_{ij} + \frac{\partial \phi}{\partial y} \bigg|_i \hat{y}_{ij} + \\
\frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_i \hat{x}^2_{ij} + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_i \hat{x}_y_{ij} + \frac{1}{2} \frac{\partial^2 \phi}{\partial y^2} \bigg|_i \hat{y}^2_{ij} + ...
\]

The mean constraint for every control volume in the the stencil \( \{V_j\}_i \) is expressed in the form given by Equation 2.16. The choice of the stencil should be compact and limited to local neighbors so that only valid data is used for reconstruction. Neighbors which are physically far from the vertex are not considered in the stencil. Using only a small topological neighborhood of a vertex ensures a compact physical support. The stencil for second order reconstruction includes the control volumes adjoining the reference control volume whereas for third and fourth order accuracy, second and third neighbors may also be included. Stencil determination is done as a pre-processing step and for control volumes which are too close to the boundary, more neighbors can be added to the stencil to have sufficient support for achieving desired accuracy of reconstruction. Once the stencil
is determined, the information from each neighbor is emphasized on the basis of proximity by using inverse distance weighting $w_{ij}$. The inverse distance weighing is used as it is observed to improve conditioning and recover accuracy in gradient calculations for isotropic meshes [25]. The resulting system of equations to be solved for the Taylor coefficients takes the form

$$
\begin{bmatrix}
1 & \bar{x}_i & \bar{y}_i & \bar{x}^2_i & \bar{x}\bar{y}_i & \bar{y}^2_i & \cdots \\
 w_{i1} & w_{i1}\bar{x}_{i1} & w_{i1}\bar{y}_{i1} & w_{i1}\bar{x}^2_{i1} & w_{i1}\bar{x}\bar{y}_{i1} & w_{i1}\bar{y}^2_{i1} & \cdots \\
 w_{i2} & w_{i2}\bar{x}_{i2} & w_{i2}\bar{y}_{i2} & w_{i2}\bar{x}^2_{i2} & w_{i2}\bar{x}\bar{y}_{i2} & w_{i2}\bar{y}^2_{i2} & \cdots \\
 w_{i3} & w_{i3}\bar{x}_{i3} & w_{i3}\bar{y}_{i3} & w_{i3}\bar{x}^2_{i3} & w_{i3}\bar{x}\bar{y}_{i3} & w_{i3}\bar{y}^2_{i3} & \cdots \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 w_{iN} & w_{iN}\bar{x}_{iN} & w_{iN}\bar{y}_{iN} & w_{iN}\bar{x}^2_{iN} & w_{iN}\bar{x}\bar{y}_{iN} & w_{iN}\bar{y}^2_{iN} & \cdots 
\end{bmatrix}
\begin{bmatrix}
\phi \\
\frac{\partial \phi}{\partial x} \\
\frac{\partial \phi}{\partial y} \\
\frac{\partial^2 \phi}{\partial x^2} \\
\frac{\partial^2 \phi}{\partial x \partial y} \\
\frac{\partial^2 \phi}{\partial y^2} \\
\cdots 
\end{bmatrix}_i
= 
\begin{bmatrix}
\bar{\phi}_i \\
\bar{\phi}_{\bar{x}} \\
\bar{\phi}_{\bar{y}} \\
\bar{\phi}_{\bar{x}\bar{x}} \\
\bar{\phi}_{\bar{x}\bar{y}} \\
\bar{\phi}_{\bar{y}\bar{y}} \\
\cdots 
\end{bmatrix}_i
$$

(2.17)

where the line separator is used to emphasize the mean constraint applied to the system of equations to be solved using least-squares and

$$
w_{ij} = \frac{1}{|r_j - r_i|}
$$

(2.18)

is the geometric weight used. In the solver, the mean constraint is eliminated analytically and the unexhausted equations are solved in a least-squares sense for every control volume by the singular value decomposition (SVD) method.

### 2.2.2.2 Weighted Least-Squares Method

The second order weighted least-squares system is derived from the equation (2.17) which gives a comprehensive formulation to obtain higher order reconstruction for any control volume. The resulting system of equations with a mean constraint to be solved is simplified as below:

$$
\begin{bmatrix}
1 & \bar{x}_i & \bar{y}_i \\
 w_{i1} & w_{i1}\bar{x}_{i1} & w_{i1}\bar{y}_{i1} \\
 w_{i2} & w_{i2}\bar{x}_{i2} & w_{i2}\bar{y}_{i2} \\
 w_{i3} & w_{i3}\bar{x}_{i3} & w_{i3}\bar{y}_{i3} \\
 \vdots & \vdots & \vdots \\
 w_{iN} & w_{iN}\bar{x}_{iN} & w_{iN}\bar{y}_{iN} 
\end{bmatrix}
\begin{bmatrix}
\phi \\
\frac{\partial \phi}{\partial x} \\
\frac{\partial \phi}{\partial y} \\
\frac{\partial^2 \phi}{\partial x^2} \\
\frac{\partial^2 \phi}{\partial x \partial y} \\
\frac{\partial^2 \phi}{\partial y^2} \\
\cdots 
\end{bmatrix}_i
= 
\begin{bmatrix}
\bar{\phi}_i \\
\bar{\phi}_{\bar{x}} \\
\bar{\phi}_{\bar{y}} \\
\bar{\phi}_{\bar{x}\bar{x}} \\
\bar{\phi}_{\bar{x}\bar{y}} \\
\bar{\phi}_{\bar{y}\bar{y}} \\
\cdots 
\end{bmatrix}_i
$$

(2.19)

The mean constraint is applied using Gauss elimination and the set of equations takes a compact form as shown.
2.2. Solution Reconstruction

\[
\begin{bmatrix}
  w_{i1}(\hat{x}_{i1} - x_i) & w_{i1}(\hat{y}_{i1} - y_i) \\
  w_{i2}(\hat{x}_{i2} - x_i) & w_{i2}(\hat{y}_{i2} - y_i) \\
  w_{i3}(\hat{x}_{i3} - x_i) & w_{i3}(\hat{y}_{i3} - y_i) \\
  \vdots & \vdots \\
  w_{iN}(\hat{x}_{iN} - x_i) & w_{iN}(\hat{y}_{iN} - y_i)
\end{bmatrix}
\begin{bmatrix}
  \frac{\partial \phi}{\partial x} \\
  \frac{\partial \phi}{\partial y}
\end{bmatrix}_i =
\begin{bmatrix}
  w_{i1}(\overline{\phi}_1 - \overline{\phi}_i) \\
  w_{i2}(\overline{\phi}_2 - \overline{\phi}_i) \\
  w_{i3}(\overline{\phi}_3 - \overline{\phi}_i) \\
  \vdots \\
  w_{iN}(\overline{\phi}_N - \overline{\phi}_i)
\end{bmatrix}
\]  

(2.20)

For second order reconstruction, the natural choice for choosing the stencil would be all the vertex neighbors connected by edges to the reference vertex, which in general vary from 5-7 for a triangular mesh and 4 for a quadrilateral mesh. The details of stencil selection, differences in stencil choice for triangular and mixed meshes, and interior and boundary control volumes are presented in the Section 2.2.3.

2.2.2.3 Advantages of Least-Squares Method

Using the least-squares method of reconstruction offers advantages and simplifications when compared to the Green-Gauss method. The reconstruction is grid transparent in the sense that it does not rely on the mesh type; whether it is a quadrilateral or a triangular mesh. The set of equations solved are related to a stencil which identifies relevant neighboring points for the reconstruction. Although the choice of stencil can be arbitrary, the most obvious choice is the set of control volumes adjacent or physically closer to the reference point. The least-squares method can be extended to calculate higher order derivatives and successively a higher order solution reconstruction which can be used to calculate both the advective and diffusive fluxes. On the other hand, the Green-Gauss method has been used predominantly for viscous fluxes along with additional schemes for calculating inviscid fluxes. The extension of the Green-Gauss method beyond second order accuracy is rarely explored. Thus the least-squares method has the benefit of providing with a single reconstruction that can be used for calculating both the inviscid and diffusive fluxes.

Further advantages are discussed in later sections where we show methods to apply boundary constraint and the use of jump terms (discussed in section 2.3.1) which are proven to be crucial in our objective of reducing truncation and discretization errors. The boundary constraints, applied at the Gauss quadrature points are such that the reconstructed solution satisfies the boundary condition exactly at the quadrature points. The Green-Gauss and least-squares methods were found to have comparable accuracies in reconstruction for isotropic meshes [25], [17] but for anisotropic meshes, the gradients were found to be inaccurate. The reader is
2.2. Solution Reconstruction

directed to the works of Jalali and Ollivier-Gooch [20] for details about accurate reconstruction on unstructured anisotropic meshes for second, third and fourth order accurate schemes using weighted and unweighted least-squares method.

2.2.3 Reconstruction Stencils

Barth and Frederickson [3] and Ollivier-Gooch [31] highlight the importance of choosing a compact support implying that the reconstruction should use data from a stencil whose members are physically and topologically closer. The size of such a stencil is defined by the number of derivatives to be evaluated, usually larger by a certain factor for least squares problem. Including additional neighbors allows leeway for ignoring non-smooth data as well. For second order accuracy, the first vertex neighbors are usually sufficient, whereas for third and fourth order accuracy, the second or third neighbors may be included. Using second neighbors is sufficient for reconstruction up to fourth order for interior control volumes but not for boundary control volumes. Quite often, an additional layer of neighbors are added for boundary control volumes to provide the necessary support.

The nearly symmetric position of the stencil neighbors pave the way for error calculation on all the sides of a control volume in the interior. In an equilateral triangular mesh or a quad mesh with rectangular elements, the cancellation is exact which yields higher orders of truncation error. Perturbed meshes exhibit lower orders of truncation error while the boundary control volumes with stencil members dominant on one side have higher error magnitudes. Lack of symmetry can also be observed in the interface layers of mixed meshes where the truncation error is also of lower order.

The choice of stencil shown in the Figure 2.3 for triangular and mixed meshes highlight the members needed for different levels of accuracy. The red marked neighbors for second order reconstruction are the first neighbors which share the boundary edges of the control volume. Hence we have four neighbors for a triangular boundary element and three for a quad boundary element. Also notice that the interface layer control volumes where the triangular and quad layer meet have about five neighbors. The stencil choice for third and fourth order reconstruction for interior control volumes coincide whereas for the boundary control volumes, the third neighbors are required for fourth order accuracy. The use of 3, 8 and 14 neighbors for second, third and fourth order accuracy, (to calculate 2, 5 and 9 derivatives) seem to be sufficient [31].
2.2. Solution Reconstruction

(a) Stencil Selection for pure triangular mesh

(b) Stencil selection for mixed mesh

Figure 2.3: Stencil choices for reconstruction
2.3 Flux Evaluation

2.3.1 Numerical Flux Calculation

Evaluation of numerical flux is a two part problem: firstly the solution reconstruction at the edge Gauss points must be performed and secondly ensuring that the flux across the edge is same for the control volumes sharing the edge. Previous sections have shown methods of solution reconstruction using least-squares and Green-Gauss methods. This section explains the methods for calculating numerical flux for the two reconstruction methods such that flux across the edge is unique.

In the least-squares reconstruction method, the gradients at the edge are not the same. Hence to calculate the flux, the gradients need to be averaged. Jalali [17] has performed multiple tests for assessing different averaging methods, addition of finite difference terms and jump terms for the calculation of face gradients to evaluate diffusive fluxes. The analysis has favored the use of linear and arithmetic averaging for gradient calculation and found them to be comparably less erroneous than volume weighted averaging. The results also found linear interpolation to be marginally better than arithmetic averaging for cell-centered schemes. The inclusion of jump terms also reduces the errors.

To evaluate the numerical flux, we perform the solution reconstruction. Once the Taylor polynomial for reconstruction is evaluated, as elaborated in Section 2.2, the gradient for the control volume can be approximated as

$$\nabla \phi^R_i(x, y) = \left( \begin{array}{c} \frac{\partial \phi}{\partial x} \bigg|_{i} + \frac{\partial^2 \phi}{\partial x^2} \bigg|_{i} (x-x_i) + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_{i} (y-y_i) + \cdots \\ \frac{\partial \phi}{\partial y} \bigg|_{i} + \frac{\partial^2 \phi}{\partial y^2} \bigg|_{i} (y-y_i) + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_{i} (x-x_i) + \cdots \end{array} \right) \quad (2.21)$$

Equation 2.21 is a general form for evaluating the gradients. For second order accurate reconstruction where the solution varies linearly in the control volume, the gradients are constant over the control volume. The need for averaging of gradients arises only when there is a discontinuity in gradients across the control volume boundaries, as is the case for least-squares reconstruction. In our research, we use both linear interpolation and arithmetic averaging to calculate the face gradients at the control volume boundaries. The averaged gradient at the flux integration Gauss point $g$ (see Figure 2.4) is shown in Table 2.1 for arithmetic and linear interpolation methods.

A damping term based on the jump in solutions across the edge was proposed by Nishikawa [30] and was found to be effective in high frequency error damping. This has been demonstrated to give more accurate solutions for diffusion problems.
2.3. Flux Evaluation

<table>
<thead>
<tr>
<th>Averaging Method</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Arithmetic Averaging (AA)</td>
<td>$\frac{1}{2} \nabla \phi_i + \frac{1}{2} \nabla \phi_j$</td>
</tr>
<tr>
<td>Linear Interpolation (LI)</td>
<td>$\frac{</td>
</tr>
</tbody>
</table>

Table 2.1: Face gradient calculation

![Figure 2.4: Linear interpolation method for numerical flux](image)

on isotropic and anisotropic meshes for cell-centered [17] and vertex-centered [45] schemes. In some cases, the lack of a damping term leads to unstable or inconsistent results. This term can be efficiently and systematically integrated with an advection scheme to solve advection-diffusion problems. The damping term, also known as jump term, is added to the averaged flux in the face normal direction as

$$\nabla \phi_{Jump} = \alpha \frac{\mathbf{r}_{ij} \cdot \mathbf{n}_F}{|\mathbf{r}_{ij} \cdot \mathbf{n}_F|} (\phi^R - \phi^L) \hat{n}_F$$  (2.22)

where $\mathbf{r}_{ij}$ is the vector joining the reference centers of the two control volumes and $\mathbf{n}_F$ is the face normal at the Gauss point $g$. The left and right control volume solutions at the Gauss point are $\phi^L$ and $\phi^R$. The jump coefficient $\alpha$ plays an important role in controlling the damping effect of the jump term. Certain values of $\alpha$ are found to increase the order of accuracy for truncation errors on uniform meshes, and in general reduce the errors in truncation and discretization significantly.

The calculation of numerical flux has been focused on using the least-squares gradient reconstruction so far. However, the Green-Gauss method presents a rather simple approach to calculate the numerical flux. Since the gradient in the primal cells is constant, the gradient across the dual edges of control volumes is the same on both sides and hence the numerical flux is the dot product of the gradient and unit normal to the edge. For instance, the numerical flux for each of the edges
2.3. Flux Evaluation

Figure 2.5: Numerical flux calculation for Green-Gauss method

of control volumes 0, 1, 2 in the primal triangular cell shown in the Figure 2.5 is simply the dot product of gradient of the cell calculated by the formula given in Equation 2.3 with the unit normal for corresponding dual edges in the primal cell.

2.3.2 Flux Integration

Discretized equations of the form given in Equation 2.1 are to be evaluated for every control volume in the mesh. The accuracy of solution hinges on the accuracy of the flux integral which in turn depends on the numerical flux accuracy and integration methods. Gauss quadrature rules of integration are used to calculate flux integral of desired accuracy. The quadrature rules calculate high order accurate flux integrals by evaluating the integrand at the Gauss points and by multiplying them with appropriate weights.

To obtain a second order accurate flux integral over a single edge, the numerical flux is evaluated at the mid point of the edge and multiplied by the edge length. A higher order flux integral needs more than one Gauss point. Figure 2.6 gives an illustration of the Gauss quadrature points. The flux integral for a control volume is a direct summation of the integration on each edge. Detailed information about the Gauss points and the appropriate weights for integration can be found in the works of Ollivier-Gooch and Van Altena [34] and Van Altena [43].

Once the flux integral is calculated for every control volume, we obtain a system of linear equations which can be solved by any matrix solution technique to obtain the steady state Poisson solution.
2.4 Boundary Treatment Methods

The boundary control volumes differ from the interior ones in two major aspects; the stencil and the application of boundary conditions. They are also the regions of a mesh where the error is maximum compared to the interior and hence need to be treated differently. Thus more resources need to be spent for an effective implementation of boundary conditions for an accurate solution. We present different methods of boundary treatments applied in our work to assess their effect on improving accuracy in truncation and discretization error. The Poisson problem is solved using a homogeneous or non-homogeneous Dirichlet boundary condition. The treatment focuses on four different approaches to reduce the error: 1) improving gradient calculation by inclusion of the boundary constraints 2) including more stencil members to increase the support for least squares method 3) applying boundary condition by using ghost cells and 4) by using jump terms.

2.4.1 Use of Hard Constraints

Equation 2.19 for least-squares reconstruction includes the mean constraint. For a boundary control volume with four members in the stencil the equation takes the form
2.4. Boundary Treatment Methods

The gradients calculated by using these set of equations with just the mean constraint weakly satisfy the boundary condition. This method of boundary treatment is termed as 'Weak Boundary Condition (WBC)' and has a jump in the reconstructed boundary solution and the given boundary condition at the Gauss point. The truncation errors are generally higher and best suited for using along with a jump term.

2.4.1 Strong Boundary Condition

Ollivier-Gooch and Van Altena [34] proposed the method of using constraints at the boundary Gauss points to satisfy the boundary condition exactly. In this way, the flux integral accurately reflects the true boundary condition. The constraint is included in the reconstruction matrix and is termed as 'Gauss Constraint'. We have two Gauss points on the boundary per control volume, one per edge on either side of the vertex for calculating second order accurate flux integral. The reconstruction matrix with the constraints at Gauss points \(G_1(x_{g1}, y_{g1})\) and \(G_2(x_{g2}, y_{g2})\) and boundary condition given by the function \(f_B(x, y)\) is

\[
\begin{bmatrix}
1 & \bar{x}_i & \bar{y}_i \\
1 & x_{g1} - x_i & y_{g1} - y_i \\
1 & x_{g2} - x_i & y_{g2} - y_i \\
w_{i1} & w_{i1}\bar{x}_{i1} & w_{i1}\bar{y}_{i1} \\
w_{i2} & w_{i2}\bar{x}_{i2} & w_{i2}\bar{y}_{i2} \\
w_{i3} & w_{i3}\bar{x}_{i3} & w_{i3}\bar{y}_{i3} \\
w_{i4} & w_{i4}\bar{x}_{i4} & w_{i4}\bar{y}_{i4}
\end{bmatrix}
\begin{bmatrix}
\phi \\
\phi_x \\
\phi_y \\
\phi_{1x} \\
\phi_{2x} \\
\phi_{3x} \\
\phi_{4x} \\
\phi_{1y} \\
\phi_{2y} \\
\phi_{3y} \\
\phi_{4y}
\end{bmatrix} = 
\begin{bmatrix}
\bar{\phi}_i \\
\bar{f}_B(x_{g1}, y_{g1}) \\
\bar{f}_B(x_{g2}, y_{g2})
\end{bmatrix}
\] (2.24)

The constraints are directly used for calculating the unknown derivatives and solution variables for this scheme. This implementation is referred to as 'Strong Boundary Condition (SBC)' where the boundary condition and the control volume average are sufficient for solution reconstruction in boundary control volumes.

2.4.1.2 4-Unknown Model

Preliminary tests revealed the error in the normal derivative (say \(y\) direction) to be higher than the tangential derivative. One remedy to fix the error in the normal
2.4. Boundary Treatment Methods

derivative is to include a higher order derivative in the normal direction to increase
the accuracy. This method is termed as the 4Unk model for the four unknowns that
are solved in the reconstruction matrix with the mean and boundary constraints
applied. The set of equations, for a boundary control volume with four neighbors,
takes the form:

\[
\begin{bmatrix}
1 & x_i & y_i & y_i^2 \\
1 & x_{g1} - x_i & y_{g1} - y_i & (y_{g1} - y_i)^2 \\
1 & x_{g2} - x_i & y_{g2} - y_i & (y_{g2} - y_i)^2 \\
w_{i1} & w_{i1}x_{i1} & w_{i1}y_{i1} & w_{i1}y_{i1}^2 \\
w_{i2} & w_{i2}x_{i2} & w_{i2}y_{i2} & w_{i2}y_{i2}^2 \\
w_{i3} & w_{i3}x_{i3} & w_{i3}y_{i3} & w_{i3}y_{i3}^2 \\
w_{i4} & w_{i4}x_{i4} & w_{i4}y_{i4} & w_{i4}y_{i4}^2 \\
\end{bmatrix}
\begin{bmatrix}
\phi \\
\frac{\partial \phi}{\partial x} \\
\frac{\partial \phi}{\partial y} \\
\frac{\partial^2 \phi}{\partial y^2} \\
\end{bmatrix}
= 
\begin{bmatrix}
\phi_i \\
f_B(x_{g1}, y_{g1}) \\
f_B(x_{g2}, y_{g2}) \\
\end{bmatrix}
\]

(2.25)

The constraints are eliminated using Gauss elimination with pivoting. The resultant
system of equations are:

\[
\begin{bmatrix}
w_{i1} Y_{i1}^2 \\
w_{i2} Y_{i2}^2 \\
w_{i3} Y_{i3}^2 \\
w_{i4} Y_{i4}^2 \\
\end{bmatrix}
\begin{bmatrix}
\frac{\partial^2 \phi}{\partial y^2} \\
\end{bmatrix}
= 
\begin{bmatrix}
w_{i1} \Phi_{i1} \\
w_{i2} \Phi_{i2} \\
w_{i3} \Phi_{i3} \\
w_{i4} \Phi_{i4} \\
\end{bmatrix}
\]

(2.26)

where the calculation of the terms \( \hat{Y}_{ij}^2 \) and \( \Phi_{ij} \) is straightforward. Equation 2.26 is
first solved using the least squares method for second derivative in \( y \) and the other
gradients are calculated later from the constraint equations.

2.4.2 Increased Stencil Size

A boundary control volume is at a natural disadvantage because it has fewer neigh-
bors when compared to a well surrounded interior CV. This directly implies that the
reconstruction matrix for a boundary CV carries less information from its neigh-
borhood than its interior counterparts. Experiments were conducted to assess if
the boundary CVs can have better gradients and in turn better truncation error
by increasing the number of neighbors in the reconstruction stencil. A triangu-
lar boundary CV has four neighbors or fewer and a quad boundary CV has three
or fewer compared to their interior counterparts, which have on an average six and
four neighbors respectively. The stencil was increased to add more neighbors. The
Figure 2.7 illustrates an experiment of increasing the stencil size for triangular and
quad boundary CV.
2.4. Boundary Treatment Methods

2.4.3 Use of Single and Two Jump Terms

The use of jump terms has been discussed in Section 2.3.1 where the importance of \( \alpha \) in reducing truncation and discretization errors has been highlighted. However for boundary control volumes, the edges on the boundary are different for the calculation of numerical flux when compared to the edges which are shared by other control volumes. For interior edges the gradient and solution for two control volumes are available to calculate the flux. At the boundary however, the gradient and solution from the reference control volume is the only information available apart from the boundary condition.

One approach would be to use the jump term for interior edges of a boundary control volume with a SBC implementation for applying boundary condition. This approach is coined as the ‘Single Jump Term Method’. In an alternate approach, a jump term instead of SBC at the boundary can also be used. This approach has been shown to significantly reduce the truncation error in Chapters 4 and 5 compared to the case where there was no jump term used. For this approach, a new jump coefficient is introduced to account for the jump in satisfying the boundary condition by solution reconstruction. Thus we will have two jump coefficients, an interior jump coefficient \( \alpha \) and a boundary jump coefficient \( \alpha_B \), and hence the implementation is called as a ‘Two Jump Term Method’. The jump term for boundary edges takes the form...
2.4. Boundary Treatment Methods

\[ \nabla \phi_{\text{JumpB}} = \frac{\alpha_B}{|r_B \cdot \hat{n}_F|} (\phi^B - \phi^R) \hat{n}_F \]  

(2.27)

where \( \phi^B \) and \( \phi^R \) are the boundary condition and reconstructed solution at the Gauss point \( B \). Experiments were conducted to assess the impact of two jump term approach versus a single jump term implementation at the boundary, in improving the accuracy of truncation and discretization errors. Figure 2.8 illustrates the use of jump terms for interior and boundary dual faces.

2.4.4 Ghost Cell Methods

An intuitive way of applying the boundary condition is to extend the domain beyond the boundaries to form ghost cells. Ghost cells are attractive in the sense that they reduce the need for a special treatment of boundary control volumes. Once ghost cell control volume averages are determined using the boundary condition, they can be directly included in the framework of least-squares reconstruction. They have been employed to apply boundary conditions for complex CFD problems to improve accuracy in solution [6] and also for flux-limiting schemes [29]. A brief description of the ghost cell implementation for different boundary conditions is provided in the books of Blazek [4] and Leveque [22].

Ghost cells are virtual cells outside the physical domain but are associated with the geometric quantities like volume, area, moments etc, and the physical quantities like temperature, pressure and velocity for CFD problems, and in our case the solution values. For the vertex-centered method, two layers of ghost cells are added outside the domain. The solution values are extrapolated from the neighboring non-ghost cell control volumes such that the boundary condition is satisfied by default.
2.4. Boundary Treatment Methods

As a result, the reconstruction for boundary control volumes has a well surrounded stencil which implicitly applies the boundary condition. The flux is calculated on the physical control volume edges at the boundary. Figure 2.9 gives an illustration of the Gauss points on the boundary and the reflection of cells used to create ghost cells.

Figure 2.9: Illustration of ghost cell method
Chapter 3

Methods of Error Analysis

The steps to obtaining a finite volume solution to a Poisson problem with different boundary treatments have been laid out in the previous chapter. The study of their effect on reducing truncation error and discretization error require that both the errors are evaluated consistently and precisely. An interesting way to evaluate truncation and discretization errors for any PDE is the Method of Manufactured Solutions (MMS). These were successfully employed for assessing the magnitude of error, order of convergence and verification of the code [5, 37, 40, 9]. Using the method of manufactured solutions, the exact solutions are known and the calculation of discretization error is thus straightforward.

Truncation error measures the accuracy of the discrete approximation to the differential equation. The truncation error analysis approach in this thesis is similar to the work of Jalali [17], where the method is applicable to any arbitrary solution. The Taylor polynomial coefficients associated with the solution and its derivatives are calculated for both the exact and numerical flux integrals and the truncation error is computed by subtracting the exact flux integral from the numerical cell residual.

The modeled Poisson’s equation is linear in nature and since we are only interested in the spatial accuracy of the discretization schemes, its steady state form alone is considered. Truncation error analysis is performed on both the linear algebra system and the numerical simulation code ANSLib whereas the calculation of discretization error is only possible on ANSLib. Both the codes are grid transparent and are capable of reading mixed meshes which are used in the course of this research. ANSLib uses an edge based data structure which allows it to handle structured, unstructured and hybrid meshes seamlessly.

The linear algebra system uses a regular topology uniform mesh which has been perturbed, scaled, sheared, stretched or curved to evaluate the truncation error. The algebra system uses an analytic approach in calculating the truncation error and is not easily generalizable to include a general unstructured mesh which has irregular connectivity of five, six or seven incident edges on a vertex. The type of mesh used for analytic tests is shown in Figure 3.1, which is primarily employed for truncation error analysis of the pure triangular mesh. A different mesh (see Figure 3.3) with quad layers in the bottom half and triangular mesh in the top half is used
3.1 Analytic Tests

The analytical approach for truncation error is explained using the Figures 3.1 and 3.3 for the interior, interface and boundary layer control volumes. The mesh is composed of equilateral triangles and quadrilaterals which have side length $h$. Truncation error analysis for interior control volume is performed on CVs whose first and second neighbors are not boundary control volumes. However, the interface layer where a triangular cell and quadrilateral cell adjoin is treated differently from an interior control volume. The control volumes on the boundary and their immediate neighbors are considered crucial for the purpose of reducing inaccuracy in boundary condition implementation and reducing truncation and discretization errors. The methodology itself reveals the differences in order of accuracy not just because of the boundary condition but also due to non-uniformity of the control for truncation error analysis of mixed meshes. The regions of concern for this mesh are the triangular-quad interface layer control volume, and the boundary quad cells. The mesh is chosen so as to include control volumes for boundary and interior quad duals, and an interface layer control volume to perform the analysis required. The numerical approach used for truncation error analysis on ANSLib can easily calculate the truncation error for any arbitrary stencil in a general unstructured mesh regardless of the partial differential equations for linear problems.
3.1. Analytic Tests

The Poisson’s equation is the model equation for diffusion problems. The computation of diffusive fluxes is a step by step procedure where the control volume averages are first conserved and the property is used for the calculation of least-squares reconstruction. Alternatively, Green-Gauss method is used for evaluating the gradients. Finally the gradients are averaged on the dual edges for the flux calculation. The benefit of analytic tests lies in a quick and easy evaluation of order of accuracy for gradient, solution and flux integral calculation.

\[
\bar{\phi}_i = \phi_i + \frac{\partial \phi}{\partial x} |_{\bar{x}_i} + \frac{\partial \phi}{\partial y} |_{\bar{y}_i} + O(h^2)
\]  

(3.1)

Consider Equation 3.1 which gives the control volume average for the vertex \(i\). For cell-centered schemes, the first moments \(\bar{x}_i\) and \(\bar{y}_i\) are both zero and by default the average is represented with second order accuracy at the centroid of the cell. However, for a vertex-centered scheme, the first moments are zero for a uniform mesh but not when the mesh is perturbed randomly. This difference plays a crucial role for analytic test accuracy. The least-squares method of reconstruction for an interior and boundary CV are presented here. As the stencil is of regular connectivity, the interior and boundary control volumes have six and four neighbors respectively.

\[
\begin{bmatrix}
  w_{i2}(\bar{x}_{i2} - \bar{x}_i) & w_{i2}(\bar{y}_{i2} - \bar{y}_i) \\
  w_{i3}(\bar{x}_{i3} - \bar{x}_i) & w_{i3}(\bar{y}_{i3} - \bar{y}_i) \\
  w_{i4}(\bar{x}_{i4} - \bar{x}_i) & w_{i4}(\bar{y}_{i4} - \bar{y}_i) \\
  w_{i5}(\bar{x}_{i5} - \bar{x}_i) & w_{i5}(\bar{y}_{i5} - \bar{y}_i) \\
  w_{i6}(\bar{x}_{i6} - \bar{x}_i) & w_{i6}(\bar{y}_{i6} - \bar{y}_i) \\
  w_{i7}(\bar{x}_{i7} - \bar{x}_i) & w_{i7}(\bar{y}_{i7} - \bar{y}_i)
\end{bmatrix}
\begin{bmatrix}
  \frac{\partial \phi}{\partial x} \\
  \frac{\partial \phi}{\partial y}
\end{bmatrix}
_i = 
\begin{bmatrix}
  w_{i2}(\bar{\phi}_2 - \bar{\phi}_i) \\
  w_{i3}(\bar{\phi}_3 - \bar{\phi}_i) \\
  w_{i4}(\bar{\phi}_4 - \bar{\phi}_i) \\
  w_{i5}(\bar{\phi}_5 - \bar{\phi}_i) \\
  w_{i6}(\bar{\phi}_6 - \bar{\phi}_i) \\
  w_{i7}(\bar{\phi}_7 - \bar{\phi}_i)
\end{bmatrix}
\]

(3.2)

The gradient of the control volume \(i = 1\) as depicted in Figure 3.1 is calculated using Equation 3.2. The uniform nature of the mesh can be seen in the calculation of the moments and weights and this results in perfect error calculation for accurate results. The gradient calculated is expressed in terms of the neighboring control volume averages as

\[
\tilde{\nabla} \phi_1 = \begin{bmatrix}
  \frac{\partial \phi}{\partial x} \\
  \frac{\partial \phi}{\partial y}
\end{bmatrix}
_i = \begin{bmatrix}
  -\frac{1}{6h}(2\bar{\phi}_7 + \bar{\phi}_2 + \bar{\phi}_6 - 2\bar{\phi}_4 - \bar{\phi}_3 - \bar{\phi}_5) \\
  \frac{\sqrt{3}}{6h}(\bar{\phi}_2 + \bar{\phi}_3 - \bar{\phi}_5 - \bar{\phi}_6)
\end{bmatrix}
\]

(3.3)
3.1. Analytic Tests

When the neighboring control volume averages are expressed as a Taylor series expansion about the reference control volume $i = 1$, the order of accuracy for the gradients can be easily assessed. The results reveal that the gradients are second order accurate for the reference control volume as shown in Equation 3.4. This order of accuracy is one more than the expected and observed order of accuracy for unstructured meshes in general.

\[
\tilde{\nabla} \phi_1 = \left( \begin{array}{c} \tilde{\frac{\partial \phi}{\partial x}} \\ \tilde{\frac{\partial \phi}{\partial y}} \end{array} \right) = \left( \begin{array}{c} \frac{23 \phi_7^2}{144} \left( \frac{\partial^3 \phi}{\partial x^3} + \frac{\partial^3 \phi}{\partial x \partial y^2} \right) + \frac{\partial \phi}{\partial x} \\ \frac{23 \phi_7^2}{144} \left( \frac{\partial^3 \phi}{\partial y^3} + \frac{\partial^3 \phi}{\partial x^2 \partial y} \right) + \frac{\partial \phi}{\partial y} \end{array} \right)
\] (3.4)

The boundary control volume has four neighbors as shown in Figure 3.2 and the neighbors differ in the moment calculation and also the type of boundary condition applied. The least-squares system for the reference control volume $i = 1$ in Figure 3.2, using weak boundary condition enforcement is given in Equation 3.5. Evidently, there is less information from the neighbors for calculating the gradients. The gradient when expressed in terms of the neighboring control volume averages is

\[
\tilde{\nabla} \phi_1 = \left( \begin{array}{c} \tilde{\frac{\partial \phi}{\partial x}} \\ \tilde{\frac{\partial \phi}{\partial y}} \end{array} \right) = \left( \begin{array}{c} \frac{1}{5h} \left( 2 \overline{\phi}_7 + \overline{\phi}_2 - 2 \overline{\phi}_4 - \overline{\phi}_3 \right) \\ \frac{\sqrt{3}}{20h} \left( \overline{\phi}_2 + \overline{\phi}_3 - 2 \overline{\phi}_1 \right) \end{array} \right)
\] (3.6)

As expected, the accuracy for boundary control volumes for gradient calculation is $O(h)$. The trend observed for the mixed cell mesh is similar for both the interior and boundary control volumes in terms of the order of accuracies for gradient calculation.

After evaluating the gradients using the least-squares method, there is a need for averaging the gradients using Table 2.1 for face gradient calculation. An example is provided for the face gradient calculation at the interface of control volumes $i = 1$ and $j = 7$ using a simple arithmetic averaging scheme for the mesh shown in Figure 3.2.
3.1. Analytic Tests

The gradient at the interface of the control volumes \(i = 1\) and \(j = 7\) lacks the symmetry which is usually observed for the interior control volumes. The face gradients and the control volume gradients are all observed to be first order accurate. Important to note is that the averaging of gradient is not required on the boundary dual edges as the boundary Gauss point lies completely within the reference control volume. Once the face gradients are calculated for every Gauss point on the control volume boundary, the flux for each dual edge is calculated by the dot product of the normal unit vector and the face gradients.

\[
\nabla \phi_{17} = \begin{pmatrix} \frac{\partial \phi}{\partial x} \\ \frac{\partial \phi}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{1}{10h}(-2\bar{\phi}_7 - 2\bar{\phi}_{18} - \bar{\phi}_{19} + \bar{\phi}_3 + 2\bar{\phi}_4 + 2\bar{\phi}_1) \\ -\frac{9\sqrt{3}}{40h}(2\bar{\phi}_7 + 2\bar{\phi}_1 - \bar{\phi}_{19} - \bar{\phi}_3 - 2\bar{\phi}_2) \end{pmatrix}
\]

(3.7)

The flux integral calculation for a dual edge is explained in Section 2.3.2 where the flux is multiplied by the appropriate weight which is the edge length for second order accuracy. Once the flux integral for the control volume is computed, we obtain an expression for the numerical flux integral in terms of the control volume averages. The numerical flux integral obtained using least-squares reconstruction is a linear combination of 19 control volumes for control volume \(i = 1\) in the Figure 3.1. Using Green-Gauss reconstruction gives a much more compact stencil for the numerical flux integral.

\[
\nabla^2 \phi_{i-LSM} = -\frac{1}{9h^2}(6\bar{\phi}_1 + \sum_{p=2}^{7} \phi_p - \sum_{q=8}^{19} \phi_q)
\]

(3.9)
3.1. Analytic Tests

![Uniform mixed cell mesh regular stencil](image)

Figure 3.3: Uniform mixed cell mesh regular stencil

\[ \overline{\nabla^2 \phi_i} - GG = -\frac{2}{3h^2} (6\overline{\phi}_1 - \sum_{p=2}^{7} \overline{\phi}_p) \quad (3.10) \]

A strong decoupling is observed when the numerical flux integral is calculated for the quad interior cells using least-squares reconstruction. A discussion of the decoupling and its effects and method to prevent decoupling can be found in the work of Haselbacher and Blazek [15]. The stencil for the flux integral is again a linear combination of 5 control volumes and doesn’t involve the immediate neighbors of the reference control volume \( i = 25 \) shown in Figure 3.3.

\[ \overline{\nabla^2 \phi_i} = \frac{1}{4h^2} (\overline{\phi}_{23} + \overline{\phi}_{27} + \overline{\phi}_{35} + \overline{\phi}_{15} - 4\overline{\phi}_{25}) \quad (3.11) \]

Decoupling can lead to spurious solution modes and large truncation errors,
3.1. Analytic Tests

both of which are undesirable. By implementing the edge derivative correction for face-gradient calculation on the dual edges (see Section 2.2.1, Equation 2.4), the numerical flux integral is recalculated using gradients calculated by least-squares method. The resultant stencil observed is a compact one involving the reference and the adjacent control volumes as shown in Figure 3.3. The numerical flux integral of an interior control volume in the quad region of the mixed mesh, calculated using least-squares method of reconstruction and edge correction for face gradients, is

\[ \hat{\nabla}^2 \phi_{i-EC} = \frac{1}{h^2} \left( \phi_{24} + \phi_{26} + \phi_{30} + \phi_{20} - 4\phi_{25} \right) \]  

(3.12)

Now that the remedies to prevent instabilities in the interior regions of the mesh are described, we proceed onto the evaluation of the flux integral for a boundary control volume. The numerical flux integral for the boundary control volume, as shown in Figure 3.2, is evaluated using least-squares reconstruction. A comparison of the stencil for interior and boundary flux integral can be drawn from the expression for the numerical flux integral for boundary given in equation below

\[ \hat{\nabla}^2 \phi_i = \frac{1}{h^2} \left( (a_1 \phi_1 + a_2 (\phi_2 + \phi_3) + a_4 (\phi_4 + \phi_7) + a_8 (\phi_8 + \phi_{10}) + a_9 \phi_9 + a_{11} (\phi_{11} + \phi_{19}) + a_{12} (\phi_{12} + \phi_{18}) \right) \]  

(3.13)

<table>
<thead>
<tr>
<th>( a_1 )</th>
<th>( a_2 )</th>
<th>( a_3 )</th>
<th>( a_4 )</th>
<th>( a_5 )</th>
<th>( a_6 )</th>
<th>( a_7 )</th>
<th>( a_8 )</th>
<th>( a_9 )</th>
<th>( a_{10} )</th>
<th>( a_{11} )</th>
<th>( a_{12} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.103</td>
<td>-1.189</td>
<td>0.319</td>
<td>-0.104</td>
<td>0.271</td>
<td>0.178</td>
<td>0.133</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3.1: Coefficients for boundary numerical flux integral

The coefficients \( a_i \)'s for Equation 3.13 are given in the Table 3.1. Even for a perfectly uniform mesh, the coefficients and a one-sided stencil hint at the lack of error cancellation required for higher order truncation error.

Having presented the stencil sizes and behavior of the schemes, we shall now discuss the evaluation of the analytic flux integrals, both exact and numerical. The evaluation of the error in the numerical flux integral requires the control volume averages in the stencil to be expressed as a Taylor series expansion about the reference control volume, using the Equation 2.16. For the purpose of demonstration, we calculate the truncation error only for the interior control volume \( i = 1 \) in Figure 3.1. The control volume averages are now replaced in Equation 3.9 by their Taylor
3.1. Analytic Tests

series expansions about the reference control volume, which after some simplification yields

\[
\bar{\nabla^2 \phi}_1 = \frac{\partial^2 \phi}{\partial x^2}_i + \frac{\partial^2 \phi}{\partial y^2}_i + \frac{41h^2}{144} \left( \frac{\partial^4 \phi}{\partial x^4}_i + 2 \frac{\partial^4 \phi}{\partial x^2 \partial y^2}_i + \frac{\partial^4 \phi}{\partial y^4}_i \right) \tag{3.14}
\]

To evaluate the truncation error, the exact flux integral has to be calculated to compare with the numerical one. The Laplacian operator is performed over the solution, which is expressed in a Taylor series expansion about its reference point as given in the Equation 2.7, and averaged over the corresponding control volume to obtain the exact flux integral. The Laplacian of the solution is given as

\[
\nabla^2 \phi_i = \frac{\partial^2 \phi}{\partial x^2}_i + \frac{\partial^2 \phi}{\partial y^2}_i + \frac{\partial^3 \phi}{\partial x \partial y^3}_i (x - x_i) + \frac{\partial^3 \phi}{\partial x^3 \partial y}_i (y - y_i) + \frac{\partial^3 \phi}{\partial x^3 \partial y}_i (x - x_i)^2 + \frac{\partial^4 \phi}{\partial x^4 \partial y^3}_i (x - x_i)(y - y_i) + \frac{\partial^4 \phi}{\partial x^4 \partial y^3}_i \left( \frac{(x - x_i)^2}{2} + \frac{(y - y_i)^2}{2} \right) + \frac{\partial^4 \phi}{\partial x^4 \partial y^3}_i (x - x_i)(y - y_i) + \frac{\partial^4 \phi}{\partial y^4}_i \left( \frac{(y - y_i)^2}{2} + \cdots \right) \tag{3.15}
\]

The next step is to take the area average over the control volume to obtain the general form of exact flux integral for arbitrary mesh.

\[
\nabla^2 \phi_i = \frac{\partial^2 \phi}{\partial x^2}_i + \frac{\partial^2 \phi}{\partial y^2}_i + \left( \frac{\partial^3 \phi}{\partial x^3 \partial y}_i + \frac{\partial^3 \phi}{\partial x \partial y^3}_i \right) \bar{x}_i + \left( \frac{\partial^3 \phi}{\partial x^3 \partial y^3}_i \bar{x}_i + \frac{\partial^4 \phi}{\partial x^4 \partial y}_i \bar{x} \bar{y}_i + \frac{\partial^4 \phi}{\partial x^4 \partial y}_i \bar{x} \bar{y}_i + \right) \left( \frac{\partial^3 \phi}{\partial x^3 \partial y^3}_i \bar{x} \bar{y}_i + \frac{\partial^4 \phi}{\partial x^4 \partial y^3}_i \bar{x} \bar{y}_i + \frac{\partial^4 \phi}{\partial y^4}_i \bar{y} \bar{x}_2 + \cdots \right) \tag{3.16}
\]

Equation 3.16 gives the exact flux integral, irrespective of whether it is a quad or a triangular control volume, interior or boundary. The moments for an interior control volume for a uniform triangular mesh are substituted in Equation 3.16 to obtain the exact flux integral.
3.2 Numerical Tests

\[ \tilde{\nabla}^2 \phi_1 = \frac{\partial^2 \phi}{\partial x^2} \bigg|_1 + \frac{\partial^2 \phi}{\partial y^2} \bigg|_1 + \frac{5h^2}{144} \left( \frac{\partial^4 \phi}{\partial x^4} \bigg|_i + 2 \frac{\partial^4 \phi}{\partial x^2 \partial y^2} \bigg|_i + \frac{\partial^4 \phi}{\partial y^4} \bigg|_i \right) + \cdots \] (3.17)

The truncation error for interior control volumes is given in Equation 3.18 which is observed to be second order accurate. If the vertex locations are perturbed randomly, this accuracy is impossible to reproduce and the truncation error stops converging with decreasing mesh size and has the order \( O(1) \).

\[ \tilde{\nabla}^2 \phi_1 - \nabla^2 \phi_1 = \frac{h^2}{4} \left( \frac{\partial^4 \phi}{\partial x^4} \bigg|_i + 2 \frac{\partial^4 \phi}{\partial x^2 \partial y^2} \bigg|_i + \frac{\partial^4 \phi}{\partial y^4} \bigg|_i \right) + O(h^4) \] (3.18)

The truncation error depends on the type of reconstruction used, face gradient calculation, use of jump terms and edge correction and also the type of boundary condition implementation. The influence of different schemes and methods on truncation error and discretization error are studied in detail in Chapters 4 and 5.

3.2 Numerical Tests

The analytic tests were designed for meshes with regular topology to give an idea about the behavior of the discretization schemes and boundary treatment methods on a topologically regular mesh. The analysis is best performed by the computer linear algebra system developed which replaces the laborious hand calculations required otherwise. A similar analysis for truncation error on general unstructured meshes is considered impractical as it would entail mathematically intense operations on every control volume. An alternative approach is explained in the following section to calculate truncation error based on the methods described by Jalali [17] for a similar analysis of cell-centered schemes in the interior regions. A brief discussion on calculation of the discretization error using the Method of Manufactured Solutions is also presented in Section 3.2.2.

3.2.1 Truncation Error

The numerical approach for calculation of truncation error is applicable for general unstructured meshes and is independent of the nature of partial differential equations solved. The approach exploits the fact that the discrete flux integral can be expressed as a linear combination of the control volume averages for an arbitrary
3.2. Numerical Tests

unstructured mesh stencil. The discrete flux integral in a general form is expressed as

$$\widetilde{\nabla^2 \phi_i} = \sum_j \frac{\partial R_i}{\partial \phi_j} \phi_j$$

where the summation is over the control volumes in the stencil \(\{V_j\}_i\) of the reference control volume \(i\). \(\frac{\partial R}{\partial \phi_j}\) is one row of the global flux Jacobian. ANSLib is capable of calculating the global flux Jacobian explicitly, for schemes up to fourth order accuracy. Detailed information on the calculation of the explicit flux Jacobian can be found in the works of Michalak [29]. The procedure pertaining to the Poisson problem is described here. The analytic Jacobian is explicitly represented as

$$\frac{\partial R}{\partial \phi} = \frac{\partial FluxInt}{\partial Var} = \frac{\partial FluxInt}{\partial Flux} \frac{\partial RecSol}{\partial RecCoef} \frac{\partial RecCoef}{\partial Var}$$

in which \(FluxInt\) is the discrete flux integral, \(Flux\) is the numerical flux calculated at the Gauss point, \(RecSol\) are the reconstructed solutions at the Gauss points, \(RecCoef\) are the coefficients of the reconstructed polynomial obtained by the least-squares method and \(Var\) is the control volume average of the unknown variable. To compute the Jacobian, the following procedure is used for each Gauss point for each of the two adjacent control volumes:

1. \(\frac{\partial RecSol}{\partial Var} = \frac{\partial RecSol}{\partial RecCoef} \frac{\partial RecCoef}{\partial Var}\) is first computed. The term \(\frac{\partial RecCoef}{\partial Var}\) is simply the pseudo-inverse of the reconstruction matrix precomputed in the least-squares system of Equation 2.17 using SVD. The numerical flux is always a function of the solution and/or solution gradient at the Gauss points and requires reconstruction of the same variables at the Gauss points. Thus \(RecSol\) is defined as \(\left( \phi \ \frac{\partial \phi}{\partial x} \ \frac{\partial \phi}{\partial y} \right)^T\). The term \(\frac{\partial RecSol}{\partial RecCoef}\) is essentially a geometric term that only depends on the location of the Gauss point, as \(RecSol\) is expressed as a Taylor polynomial about the reference point.

2. In the Poisson problem, the Flux is defined as the dot product of the face gradients and the unit normal vector at the Gauss points. Thus \(\frac{\partial Flux}{\partial RecSol}\) depends on the choice of discretization and use of jump terms or edge derivative correction to calculate the flux. So if only arithmetic averaging is used for
3.2. Numerical Tests

Calculating the face gradient, the term evaluates as

\[
\frac{\partial \text{Flux}}{\partial \text{RecSol}_L} = \frac{\partial \text{Flux}}{\partial \text{RecSol}_R} = \begin{pmatrix} 0 & -\frac{1}{2} \hat{n}_x & -\frac{1}{2} \hat{n}_y \end{pmatrix}
\]  

(3.21)

3. \( \frac{\partial \text{FluxInt}}{\partial \text{Flux}} \) depends on the Gauss quadrature formula. It is calculated by using the appropriate Gauss integration weight and the length of the corresponding edge.

4. After calculating all the terms, the \( \frac{\partial \text{FluxInt}}{\partial \text{Var}} \) is obtained by combining them.

Once the explicit Jacobian \( \frac{\partial \phi}{\partial \varphi} \) is calculated using the above procedure\(^1\), the steps to express the flux integral in terms of the control volume averages \( \bar{\phi}_j \) is performed. Then, the control volume averages for the neighboring control volumes are replaced by their Taylor series expansions about the reference control volume in terms of its solution and derivatives, using Equation 2.16. In calculating the sum, the terms corresponding to the Taylor coefficients are collected so as to attain a form seen in numerical flux integral given by the Equation 3.14. The exact flux integral is calculated again by computing the average of the flux integral over the entire control volume as given in Equation 3.16. The difference of the numerical flux integral from the exact flux integral simply gives the truncation error for each control volume. Subject to different boundary treatments, jump terms or discretization methods, the truncation error is evaluated over the family of meshes to perform convergence and accuracy analysis for various schemes.

3.2.2 Discretization Error

Discretization error is usually difficult to measure for general flow scenarios, especially when the exact solution is unknown. Roy [36] has reviewed different discretization error estimators and noted that these estimations are only reliable when the numerical solution is in asymptotic range, the verification of which requires at least three systematically refined meshes. It has also been observed [12] that for regular grids, the convergence of truncation error is an accurate indicator of convergence for discretization errors provided the discrete boundary conditions are adequate. On irregular grids, though, the truncation error convergence is not a good predictor for discretization error convergence. Design order discretization error convergence has been observed in cases where the truncation error converges

\(^1\)An alternative way to calculate the Jacobian is the “finite difference Jacobian” where the variables concerned are perturbed individually and the change in the flux integral function is measured to calculate the Jacobian. This method is slower than explicit Jacobian method and is used for truncation error estimation using the Green-Gauss reconstruction scheme.
3.2. Numerical Tests

at a lower than expected order or doesn’t converge at all. Thus it’s necessary to estimate the discretization error accurately and study its relationship with truncation error.

Given the simple nature of Poisson’s equation, we use the Method of Manufactured Solutions with three exact solutions and the associated source terms to solve the problem numerically. The discrete solution obtained is then compared with the exact solution to evaluate the discretization error. To verify the convergence order of discretization error, we use four systematically refined meshes for each sequence of mesh type. The relationship between the truncation error and discretization error is explored and the effect of different discretization schemes and boundary treatment methods are analyzed for reducing discretization error as well. An attempt is also made to realize the conditions under which the truncation error and discretization error are minimized simultaneously. The effects of minimizing truncation error and its influence on discretization error are also studied.
Chapter 4

Triangular Mesh Results

To achieve the least truncation error at the boundary with reduced discretization error, we proceed in a step-by-step manner. The schemes presented in Section 2.4 are subjected to analytic tests described in Section 3.1 and those that perform well are implemented in the unstructured solver. Numerical tests are then performed to confirm the behavior observed in analytic tests and to generalize the results for isotropic unstructured meshes. Using analytic tests, we exploit the algebraic nature of results to estimate the order of convergence for truncation error for various discretization schemes and boundary treatment methods, and the order of error in gradient calculation for different reconstruction methods. This gives a prediction for the behavior to be expected in the unstructured solver, paving the way to verify and solve the problem accurately.

The analytic tests for triangular meshes are performed on the meshes shown in Figures 3.1 and 3.2 for interior and boundary control volumes. Using the same topology, the mesh is perturbed in many systematic and random ways to test for different cases. The schemes performing poorly are eliminated from consideration for numerical tests where the mesh is fully unstructured. The following sections detail the findings of analytic tests followed by numerical tests performed on purely triangular meshes.

4.1 Analytic Test Analysis

Analytic tests provide an excellent analysis method to verify if the reconstruction, face-gradient calculation and flux integration behave the way as expected. As highlighted earlier, they are used to troubleshoot errors in implementation and also predict the behavior of schemes on general unstructured meshes. To ensure that analytic results are applicable for general scenarios, they are tested on five topologically regular meshes, which are created by distorting the vertices of a uniform triangular mesh in a specific manner and are shown in Figure 4.1. The reference position for \( CV_1 \) is preferably but not necessarily kept at the origin. The family of distorted meshes are described here:

1. Sheared meshes are distortions of a uniform triangular mesh where the y-
coordinates remain unchanged but the x-coordinates are sheared. The x-coordinates in a horizontal line are all moved by a constant factor which is a function of their distance from the reference x-axis. If each horizontal line is numbered with the reference x-axis as 0th row and increasing upwards, the new x-coordinates are then obtained by adding a constant amount $bmh$ where $b > 0$ is a constant shearing factor and $m$ is the row number. The new x-coordinates are such that the slanted lines remain straight and parallel.

2. Scaled meshes have the x-coordinates of a uniform mesh unperturbed but the y-coordinates are scaled by a constant factor of $k > 0$.

3. Stretched meshes also have the x-coordinates the same as that of uniform mesh. However, the y-coordinates appear stretched as one moves away from the reference x-axis. A stretching factor $s$ is defined to determine the height of each row of vertices. If the horizontal rows are numbered, the height of the triangle between rows $m + 1$ and $m$ would be given by $\frac{\sqrt{3}}{2}hs^{-m}$, where $0 < s < 1$.

4. Curved meshes are such that the mesh vertices are all transformed to a radial coordinate system. The vertices with the same y-coordinate are mapped onto a circular arc with the same radial coordinate while the vertices with the same x-coordinate are mapped on the radial line with the same polar angle $\theta$. These meshes are characterized by the constant ratio ($R$) of radius between the consecutive layers of mesh and by the ratio $a = \frac{L}{r_0}$ for the mesh.

5. Random meshes have both the coordinates of the vertices perturbed randomly, by $\rho_xh$ and $\rho_yh$ in the x and y directions respectively. The random variations $\rho_x, \rho_y \in [-0.1, 0.1]$ such that the resultant mesh has non-overlapping cells after the operation.

### 4.1.1 Reconstruction Accuracy

A first order gradient is expected for a second order solution reconstruction using the least-squares and the Green-Gauss method. As discussed earlier, the gradients for a control volume calculated by the least-squares method involve solving the system of equations required to minimize the error in satisfying the mean in neighboring control volumes. The Green-Gauss method calculates the gradient for the primal cell instead of the control volume itself. Both the methods calculate the gradients as a linear combination of control volume averages in the stencil of the reference CV.
4.1. Analytic Test Analysis

We have already discussed the gradient accuracy for interior control volumes for a perfect mesh which has second order accuracy for reconstruction. We now observe the gradient accuracy for control volumes in the stencil of the reference boundary control volume $i = 1$ in the Figure 3.2, using the least-squares reconstruction. The evaluation of the gradients is explained in Section 3.1 on page 38 and the same results are presented here:

$$
\tilde{\nabla} \phi_1 = \begin{pmatrix}
\frac{\partial \phi}{\partial x} \\
\frac{\partial \phi}{\partial y}
\end{pmatrix}
= \begin{pmatrix}
\frac{-\frac{1}{5h} \left(2\Phi_7 + \Phi_2 - 2\Phi_4 - \Phi_3\right)}{20h} \\
\frac{9\sqrt{3}}{20h} \left(\Phi_2 + \Phi_3 - 2\Phi_1\right)
\end{pmatrix}
$$
(4.1)

$$
= \begin{pmatrix}
\frac{\partial \phi}{\partial x} \bigg|_1 + \frac{11\sqrt{3}}{54} \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_1 & h + O(h^2) \\
\frac{\partial \phi}{\partial y} \bigg|_1 + \frac{9\sqrt{3}}{80} \left(\frac{\partial^2 \phi}{\partial x^2} \bigg|_1 + 3 \frac{\partial^2 \phi}{\partial y^2} \bigg|_1\right) & h + O(h^2)
\end{pmatrix}
$$
Equation 4.1 gives the gradient calculated for a boundary control volume of the uniform mesh. The control volume averages in the above gradient calculation are expressed as a Taylor series expansion about the reference control volume \( i = 1 \) using the Equation 2.16, to determine its accuracy. The Taylor series expansion of the solution variable about the control volume reference point is given as:

\[
\phi_i(x, y) = \phi_i + \frac{\partial \phi}{\partial x} \bigg|_i (x - x_i) + \frac{\partial \phi}{\partial y} \bigg|_i (y - y_i) + \\
\frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} \bigg|_i (x - x_i)^2 + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_i (x - x_i)(y - y_i) + \\
\frac{1}{2} \frac{\partial^2 \phi}{\partial y^2} \bigg|_i (y - y_i)^2 + \ldots
\]

To calculate the exact gradient, the Del operator is performed over the above equation. The resultant is averaged over the control volume to calculate the exact gradients as shown:

\[
\nabla \phi_i = \left( \begin{array}{c}
\frac{\partial \phi}{\partial x} \\
\frac{\partial \phi}{\partial y}
\end{array} \right)_i = \left( \begin{array}{c}
\frac{\partial \phi}{\partial x} \bigg|_i + \frac{\partial^2 \phi}{\partial x^2} \bigg|_i \bar{x}_i + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_i \bar{y}_i + \cdots \\
\frac{\partial \phi}{\partial y} \bigg|_i + \frac{\partial^2 \phi}{\partial y^2} \bigg|_i \bar{y}_i + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_i \bar{x}_i + \cdots
\end{array} \right)
\]

The difference in the exact and discrete gradient calculation gives the cell gradient error and one can verify the order of accuracy for reconstruction from this error. The general form of this error is:

\[
\vec{\nabla} \phi_i - \nabla \phi_i = \left( \begin{array}{c}
\left( \vec{\xi}_x \frac{\partial \phi}{\partial x} \bigg|_1 + \vec{\xi}_y \frac{\partial \phi}{\partial y} \bigg|_1 \right) + \\
\left( \frac{\partial^2 \phi}{\partial x^2} \bigg|_1 \vec{\xi}_{xx} + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_1 \vec{\xi}_{xy} + \frac{\partial^2 \phi}{\partial y^2} \bigg|_1 \vec{\xi}_{yy} \right) h + O(h^2)
\end{array} \right)
\]

\[
\left( \begin{array}{c}
\eta_x \frac{\partial \phi}{\partial x} \bigg|_1 + \eta_y \frac{\partial \phi}{\partial y} \bigg|_1 \\
\left( \frac{\partial^2 \phi}{\partial x^2} \bigg|_1 \eta_{xx} + \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_1 \eta_{xy} + \frac{\partial^2 \phi}{\partial y^2} \bigg|_1 \eta_{yy} \right) h + O(h^2)
\end{array} \right)
\]
## 4.1. Analytic Test Analysis

### Table 4.1: Gradient error coefficients for boundary control volumes

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\xi_x$</th>
<th>$\xi_y$</th>
<th>$\xi_{xx}$</th>
<th>$\xi_{xy}$</th>
<th>$\xi_{yy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Least-Squares</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<td>0</td>
<td>0</td>
<td>0.1283</td>
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</tr>
<tr>
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<td>0.00208</td>
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<tr>
<td>Green-Gauss</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<td>0</td>
<td>0</td>
<td>0.64150</td>
<td>0</td>
</tr>
<tr>
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<td>−0.00816</td>
<td>−0.46849</td>
<td>−0.00608</td>
<td>−0.00191</td>
</tr>
</tbody>
</table>

(a) Error coefficients of $\frac{\partial \phi}{\partial x}$

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\eta_x$</th>
<th>$\eta_y$</th>
<th>$\eta_{xx}$</th>
<th>$\eta_{xy}$</th>
<th>$\eta_{yy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Least-Squares</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>0</td>
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<td>0.19486</td>
<td>0</td>
<td>0.36004</td>
</tr>
<tr>
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<td>0</td>
<td>0.18030</td>
<td>−0.00084</td>
<td>0.37131</td>
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<tr>
<td>Green-Gauss</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<td>−0.35668</td>
<td>0.21764</td>
</tr>
</tbody>
</table>

(b) Error coefficients of $\frac{\partial \phi}{\partial y}$

### Table 4.2: Gradient error coefficients for interior control volumes

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\xi_x$</th>
<th>$\xi_y$</th>
<th>$\xi_{xx}$</th>
<th>$\xi_{xy}$</th>
<th>$\xi_{yy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Least-Squares</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>0</td>
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</tr>
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<td>Random</td>
<td>0</td>
<td>0</td>
<td>0.09227</td>
<td>0.070601</td>
<td>−0.00856</td>
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<tr>
<td>Green-Gauss</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<td>0</td>
<td>0</td>
<td>0.86603</td>
<td>0</td>
</tr>
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<td>Random</td>
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<td>−0.01254</td>
<td>1.04424</td>
<td>0.02339</td>
</tr>
</tbody>
</table>

(a) Error coefficients of $\frac{\partial \phi}{\partial x}$

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\eta_x$</th>
<th>$\eta_y$</th>
<th>$\eta_{xx}$</th>
<th>$\eta_{xy}$</th>
<th>$\eta_{yy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Least-Squares</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<td>0.12935</td>
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<td>Green-Gauss</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>0.47531</td>
</tr>
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<td>0.12362</td>
<td>0.02548</td>
<td>0.47531</td>
</tr>
</tbody>
</table>

(b) Error coefficients of $\frac{\partial \phi}{\partial y}$

Table 4.1: Gradient error coefficients for boundary control volumes

Table 4.2: Gradient error coefficients for interior control volumes
Tables 4.1 and 4.2 give the error coefficients $\xi$ and $\eta$ for gradients as in Equation 4.4 for a random mesh with fixed perturbations. The least-squares method of reconstruction performs the way as expected with the error coefficients for the zero order error being zero ($\xi_x = \xi_y = 0$ and $\eta_x = \eta_y = 0$). The Green-Gauss method follows this trend only for perfect and non-randomly perturbed meshes, in the interior control volumes. The Green-Gauss method as discussed in the Section 2.2.1 yields a zero-order gradient for general random meshes and is thus undesirable.

The error metrics for interior control volumes are given for comparison and one can notice that the gradient for the least-squares method is one order better for uniform interior control volumes than expected and has a minimum of first order accuracy for all other cases, for interior and boundary control volumes. It is also important to note that the error coefficients for gradients in the normal direction $y$ to the boundary is twice the error in the tangential direction $x$ to the boundary. This result served as a motivation to improve the gradient in the normal direction and is the reason for the implementation of the method described in Section 2.4.1.2

An analysis of the results also reveal that the Green-Gauss method is under performing for random meshes in the interior and in general for boundary control volumes with the gradient being zero order. Experiments revealed that such a discrepancy arises because the control volume average is used for the gradient calculation but the reference locations used are the vertex points. This has the implication of having one order less accurate gradients as the vertex locations represent the control volume average with first order accuracy and not second order accuracy; the centroids of the control volumes do so by default. So instead of using the vertex locations, the centroid locations where used for calculating the gradients and upon verification, the gradient accuracy was found to be consistent with the expected order. The flux integration however, is performed on the same median dual for the corrected Green-Gauss method. To implement this correction, one would use the centroid locations of the corresponding control volumes as $(x_j, y_j)$ instead of the vertex locations in the Equation 2.3 to calculate the gradients. The results for corrected Green-Gauss method for interior and boundary control volumes is as shown in the Table 4.3.

The error coefficients for both the Green-Gauss methods behave identically for interior uniform mesh as it was expected. Clearly, the gradient using the reference location correction for Green-Gauss method is first order accurate, as can be seen from the Table 4.3. The gradient error coefficients are also observed to be better for the least-squares method when compared to the Green-Gauss method, with or without correction.
4.1. Analytic Test Analysis

Table 4.3: Gradient error coefficients using corrected Green-Gauss method

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\xi_x$</th>
<th>$\xi_y$</th>
<th>$\xi_{xx}$</th>
<th>$\xi_{xy}$</th>
<th>$\xi_{yy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interior control volume</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<tr>
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<td>0</td>
</tr>
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<td>0</td>
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<td>0.01655</td>
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(a) Error coefficients of $\frac{\partial \phi}{\partial x}$

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\eta_x$</th>
<th>$\eta_y$</th>
<th>$\eta_{xx}$</th>
<th>$\eta_{xy}$</th>
<th>$\eta_{yy}$</th>
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<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Uniform</td>
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<td>0.19486</td>
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<td>0.36004</td>
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</table>

(b) Error coefficients of $\frac{\partial \phi}{\partial y}$

4.1.2 Flux Integral Accuracy

The truncation error for the Poisson’s equation is calculated as described in Section 3.1 where the exact flux integral is subtracted from the computed residual for the control volume. The Table 4.4 gives the results for order of truncation error with different schemes and reconstruction methods, for a variety of distorted meshes for interior and boundary control volumes. The table shows the zero order truncation error obtained for boundary control volumes using the least-squares method and the corrected Green-Gauss (GGC) method. The flux integral for the least-squares method (LSM) is calculated using both the arithmetic averaging (AA) and linear interpolation (LI) and the order of convergence was found to be identical. The Green-Gauss method without correction (GG), however, has negative order of convergence for truncation errors with curved and random meshes. The order of truncation error for LSM and corrected Green-Gauss method is in agreement with the results of Diskin and Thomas [9]. Diskin and Thomas [12] also highlight that lower order of convergence or lack of convergence doesn’t necessarily indicate that the solution doesn’t converge. In fact, the solution is found to converge for all the reconstruction methods for isotropic meshes, as shown in the numerical results in.
4.1. Analytic Test Analysis

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Boundary Mesh</th>
<th>Uniform</th>
<th>Sheared</th>
<th>Scaled</th>
<th>Stretched</th>
<th>Curved</th>
<th>Random</th>
</tr>
</thead>
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<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td></td>
</tr>
<tr>
<td>GG</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1/h)$</td>
<td>$O(1/h)$</td>
<td></td>
</tr>
<tr>
<td>GGC</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td></td>
</tr>
</tbody>
</table>

(a) Boundary control volumes

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Interior Mesh</th>
<th>Uniform</th>
<th>Sheared</th>
<th>Scaled</th>
<th>Stretched</th>
<th>Curved</th>
<th>Random</th>
</tr>
</thead>
<tbody>
<tr>
<td>LSM</td>
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<td>$O(h^2)$</td>
<td>$O(h^2)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td></td>
</tr>
<tr>
<td>GGC</td>
<td>$O(h^2)$</td>
<td>$O(h^2)$</td>
<td>$O(h^2)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td>$O(1)$</td>
<td></td>
</tr>
</tbody>
</table>

(b) Interior control volumes

Table 4.4: Truncation error order comparison for flux integral

The order of convergence for truncation error can be shown to depend on the accuracy of the gradient provided the flux integral quadrature formula is of adequate accuracy. By careful inspection of Equation 4.5, we observe that the surface area $A_{CV_i}$ and $s$ are proportional to $h^2$ and $h$, respectively. Hence if the accuracy for the gradient is first order, the flux integral has a zero order accuracy, in the absence of error cancellation. However, in case of the normal Green-Gauss method, the gradient is zero order and thus we observe a negative order of convergence for truncation errors. There are cases where the zero order terms of the flux integral cancel out resulting in a higher order truncation error. This is most commonly observed for interior control volumes when the uniform, scaled and sheared meshes were used. Such a cancellation was never observed for boundary control volumes because they lack a well surrounded stencil like the interior control volumes.

The general form of truncation error, based on the expected order of accuracy from Table 4.4, can be written as:

$$\nabla^2 \phi_i = \frac{1}{A_{CV_i}} \oint_{\partial V_i} \nabla \phi_F \cdot \hat{n} ds \quad (4.5)$$
4.1. Analytic Test Analysis

\[ \nabla^2 \phi_i - \nabla^2 \phi_i = \left( \lambda_{xx} \frac{\partial^2 \phi}{\partial x^2} \bigg|_{i} + \lambda_{xy} \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_{i} + \lambda_{yy} \frac{\partial^2 \phi}{\partial y^2} \bigg|_{i} \right) + O(h) \quad (4.6) \]

The truncation error can be calculated if the exact solution and the error coefficients are known. However, the problem of minimizing will then be dependent on the nature of problem solved. The error coefficients are the property of the stencil \( \{V_j\}_i \) specifically and generally depend on the mesh. Thus the truncation error can be minimized indirectly by minimizing the error coefficients so that the results will be applicable to any solution. A truncation error metric is used, similar to the one used by Jalali [17] to compare different schemes in their effectiveness to reduce truncation error. The error metric is the L2 norm of the error coefficients, as shown:

\[ E_i = \left( \lambda_{xx}^2 + \lambda_{xy}^2 + \lambda_{yy}^2 \right)^{\frac{1}{2}} \quad (4.7) \]

4.1.3 Boundary Treatment Methods

The error coefficients change with the change in schemes used for flux calculation, boundary treatment methods and especially with the reconstruction method. For triangular meshes, there was less scope to experiment and improve the results with the Green-Gauss method compared to the least-squares method. Using least-squares reconstruction, we can either try to increase the accuracy of the gradients, increase the stencil size or implement the boundary conditions differently. Methods like SBC and 4-Unknown models are aimed at improving the accuracy of gradients. Increasing the stencil size is also expected to improve the gradient accuracy whereas ghost cells and use of jump terms are expected to implement boundary condition effectively.

Reflecting on Section 4.1.1 and the gradient error in Equation 4.4, error metrics are defined for the gradients to compare the accuracy of different methods.

\[ EX_i = \left( \xi_{xx}^2 + \xi_{xy}^2 + \xi_{yy}^2 \right)^{\frac{1}{2}} \quad (4.8) \]

\[ EY_i = \left( \eta_{xx}^2 + \eta_{xy}^2 + \eta_{yy}^2 \right)^{\frac{1}{2}} \quad (4.9) \]

Figure 4.2 presents the results for the use of different schemes to improve the gradient at the boundary. For weak boundary condition enforcement, the error in the normal gradient is almost twice the error in the tangential gradient. The errors in the gradients are comparable for both the SBC model and the 4-Unknown models. Stencil size was increased to provide sufficient support for reconstruction of gradients. However, the increase in stencil size seems to affect the gradient
A jump term is added to the flux in the face normal direction. An interesting result is observed when a jump term is used for interior control volume on a uniform mesh. The truncation error is second order accurate when the least-squares method is used. By using a single jump term, the truncation error takes the analytic form as shown:

$$
\nabla^2 \phi_i - \nabla^2 \phi_j = \frac{3h^2}{16} \left( \frac{4}{3} - \alpha \right) \left( \frac{\partial^4 \phi_i}{\partial x^4} + 2 \frac{\partial^4 \phi_i}{\partial x^2 \partial y^2} + \frac{\partial^4 \phi_i}{\partial y^4} \right) + O(h^4)
$$

The jump coefficient modifies the error coefficients and in this case, it can increase the order of accuracy if the jump coefficient is chosen to be $\alpha = \frac{4}{3}$. The resultant truncation error is observed to be of the order of $O(h^4)$ by the use of single jump term for uniform interior control volumes. A gain in order of accuracy was impossible to achieve for a random mesh; the truncation error was however found to be reduced significantly. The truncation error for a boundary control volume, using single jump term is given as.
where \( C_{xx}, C_{yy} \) are coefficients for \( \alpha \) in the truncation error for flux integral. One intuitive way to achieve a higher order truncation error is to introduce another control variable, like the jump term \( \alpha \) in the flux calculation. Using a boundary jump term is one way to introduce the required control parameter \( \alpha_B \) through which a higher order truncation error can be achieved. The truncation error with two jump terms takes the form

\[
\widetilde{\nabla}^2 \phi_i - \nabla^2 \phi_i = \left( (\lambda_{xx} - C_{xx} \alpha) \frac{\partial^2 \phi}{\partial x^2} \right) + \left( (\lambda_{yy} - C_{yy} \alpha) \frac{\partial^2 \phi}{\partial y^2} \right) + O(h) \quad (4.11)
\]

where \( \lambda_{xx}, \lambda_{yy} \) are coefficients for \( \alpha_B \) in the truncation error for flux integral. By a careful selection of the jump coefficients it is possible to have a higher order truncation error for uniform boundary control volumes. However, the stability of the solution is a concern for the jump coefficients obtained for this case and hence, the discussion is left for future work. The corresponding error metric when jump terms are used for a regular boundary control volume is given in Equation 4.13 which predicts the behavior of the error metric to be parabolic with the variations in jump coefficients. The jump coefficient \( \alpha_B \) appears only for boundary control volumes and hence its effect is local.

\[
E_{i-\text{jump}} = \left( (\lambda_{xx} - C_{xx} \alpha - B_{xx} \alpha_B)^2 \right) + \left( (\lambda_{yy} - C_{yy} \alpha - B_{yy} \alpha_B)^2 \right) + \left( (\lambda_{yy} - C_{yy} \alpha - B_{yy} \alpha_B)^2 \right) \quad (4.13)
\]

where \( B_{xx}, B_{yy} \) are the corresponding coefficients for \( \alpha_B \) in the truncation error for flux integral. By a careful selection of the jump coefficients it is possible to have a higher order truncation error for uniform boundary control volumes. However, the stability of the solution is a concern for the jump coefficients obtained for this case and hence, the discussion is left for future work. The corresponding error metric when jump terms are used for a regular boundary control volume is given in Equation 4.13 which predicts the behavior of the error metric to be parabolic with the variations in jump coefficients. The jump coefficient \( \alpha_B \) appears only for boundary control volumes and hence its effect is local.

The performance of the boundary treatment methods are compared for a random mesh using the error metric for truncation error in the flux integral. The results are presented in the Figure 4.3. Except for the corrected Green-Gauss method, all other schemes employ the least-squares method of reconstruction. The error metric is presented on the primary axis whereas the secondary axis gives the percentage ratio for all the methods in comparison to weak boundary condition (WBC).

The Green-Gauss method follows the trend observed in the gradients where the error coefficients for the gradients were higher than the least-squares method. In this plot, the Green-Gauss method has errors almost twice the error compared
4.1. Analytic Test Analysis

Figure 4.3: Comparison of boundary treatment methods

to weak boundary condition implementation. Using ghost cells or increasing the stencil size hasn’t performed better than the weak boundary condition either. Even with an increased stencil, the errors in 4-Unknown model and SBC were higher than the normal stencil. Although the gradients were of comparable accuracy for the 4-Unknown and SBC methods, the use of the second derivative to get an accurate gradient in y at the Gauss points doesn’t improve the truncation error much. Hence, the SBC method performs better than its counterpart. Using a single and two jump term for boundary control volumes result in at least 75% reduction in truncation error. Two jump term method fares better than the single jump term method.

In view of the results for different boundary treatment methods, the use of ghost cells and the 4-Unknown model is dropped for numerical tests as the results show little promise compared to other schemes. The corrected Green-Gauss method is presented only for comparison whereas the use of SBC and jump terms is further explored, with and without the increase of stencil size. The numerical results for different reconstruction methods, gradient averaging methods and boundary treatment methods are presented in the next section.
4.2 Numerical Test Analysis

A number of different methods were tested in the previous section where some performed as expected and some underperformed. Schemes successful in reducing truncation error are now considered for the numerical tests where the truncation error is calculated for a sequence of unstructured meshes. Discretization error is also calculated by using the method of manufactured solutions, taking advantage of exact solutions satisfying Poisson’s equation to compare. Different manufactured solutions are tested to ensure that the results are applicable for a broader range of problems.

4.2.1 Isotropic Boundary Layer Mesh

A sequence of unstructured meshes were generated for a unit square domain, the coarsest and finest mesh of which are presented in the Figure 4.4. The mesh size increases such that the characteristic length halves in the sequence and the mesh is named as Sq-# where the number is approximately equal to the square root of the number of vertices. The triangular elements are of high quality and the size changes gradually across the domain. The mesh is isotropic, both in the interior and near the boundary, with an aspect ratio of about one near the boundary.

We shall discuss the convergence of the schemes to assess the order of accuracy
4.2. Numerical Test Analysis

for truncation and discretization error followed by confirmation of results observed in analytic tests with an emphasis on the flux integral and solution accuracy. To compare the truncation error, we use the error metric calculated at the control volume reference point, as the one used for analytic tests discussed in Section 4.1.2. An $L_2$ norm of error metrics for the control volumes of the mesh is used to compare the effectiveness of the schemes in achieving the set goals. However, there are two truncation error $L_2$ norms defined for a mesh, the interior and boundary. The interior error norm considers only the interior control volumes such that none of the vertex neighbors lie on the boundary. It by default excludes errors for the boundary control volumes and their first neighbors which is accounted for, by the boundary error norm. The discretization error calculation is straightforward where the control volume average of the discrete solution is compared with the exact control volume average and the $L_2$ norms for the overall mesh is used as a measure for comparison.

Figure 4.5 gives the truncation error distribution for a Sq30 mesh using least-squares method and strong boundary condition implementation. The figure validates the necessity to have a separate error norm for the boundary control volumes and their first neighbors as the magnitude of the error is higher for these control volumes. Using the strong boundary condition, the error on the boundary Gauss points is driven to zero by explicitly satisfying the boundary condition through reconstruction. This is the reason as to why the source term for solution error, which is the truncation error, has higher magnitude in the boundaries. The negative magnitude of truncation error metric near the boundary is common among different meshes and can be intuitively deduced through the relation given in the Equation 1.1.

In the previous section, the schemes which were effective in reducing truncation error were WBC, SBC, single and two jump term methods where the increased stencil size and Green-Gauss methods were used for just comparison. However, the use of WBC for boundary condition implementation alone doesn’t converge and needs the use of a jump term for convergence.

Three manufactured solutions are used for conducting the numerical tests. The first two apply homogeneous Dirichlet boundary condition whereas the third applies a non-homogenous Dirichlet boundary condition. The manufactured solutions used are shown in the Table 4.5 and presented in the Figure 4.6. The source term for each of the exact solution is manufactured by applying the Laplacian operator over the exact solution, and is fed to the numerical solver ANSLib.

The exact solution $U = -\sin(\pi x)\sin(\pi y)$ is used to conduct preliminary numerical tests and accumulate initial data for rigorous testing with other manufactured solutions. The convergence plots for discretization error is presented in the Figure 4.7 to ascertain that all the schemes have consistent order of accuracy. The least-
4.2. Numerical Test Analysis

(a) Error in second derivative of x
(b) Error in second derivative of y

Figure 4.5: Truncation error distribution for Sq30 mesh using least-squares method

<table>
<thead>
<tr>
<th>Case</th>
<th>Boundary Condition</th>
<th>Exact Solution $U$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Dirichlet Homogenous</td>
<td>$-\sin(\pi x)\sin(\pi y)$</td>
</tr>
<tr>
<td>2</td>
<td>Dirichlet Homogenous</td>
<td>$20(x - 1)(y - 1)\log(x + 1)\log(y + 1)$</td>
</tr>
<tr>
<td>3</td>
<td>Dirichlet Non-Homogenous</td>
<td>$\sin(\pi(x + y))$</td>
</tr>
</tbody>
</table>

Table 4.5: Manufactured solutions used for numerical tests

squares method results are presented for both linear interpolation and arithmetic averaging methods of face gradient calculation. Both the methods are observed to converge with second order accuracy and the difference in discretization error is also minor. A comparison with the Green-Gauss method with and without correction reveal that the latter exhibits a first order convergence when the difference in discrete and exact control volume averages are used as a measure of error. Hence for our calculations, we use only the corrected version of Green-Gauss method (GGC) for comparison and the error is always calculated by comparing discrete and exact control volume averages of the solution. The corrected Green-Gauss method appears to fare slightly better than the least-squares method with SBC when it comes to having accurate solution. Its important to note that the corrected Green-Gauss method applies the boundary flux in a way as to enforce the boundary condition value at the vertices as the control volume average. The increase in stencil neighbor size also leads to lack of convergence for least-squares method. In accordance with the convergence results obtained, the two jump term method with WBC implementation, the single jump term method, the strong boundary condi-
4.2. Numerical Test Analysis

(a) Case 1: Sinusoidal solution with homogeneous boundary

(b) Case 2: Logarithmic solution with homogeneous boundary

(c) Case 3: Sinusoidal solution with non homogeneous boundary

Figure 4.6: Exact solutions used for discretization error analysis
4.2. Numerical Test Analysis

Figure 4.7: Convergence plots for discretization errors

tion, and the corrected Green-Gauss method are the only methods used for testing numerically. Experiments with increased stencil are few and shown to confirm the observations found in analytical results. Unless specified, the face gradients are averaged by linear-interpolation.

Figure 4.8 presents the results for the use of a single jump term with a strong boundary condition applied at the boundary. The error metric corresponding to $\alpha = 0$ is equivalent to using only the SBC implementation for boundary. Observing both the figures, we can deduce that the use of jump terms effectively reduces the truncation error for interior and boundary control volumes. The truncation error with jump terms is lower than the case with SBC, confirming the better performance of jump terms over SBC. The jump coefficient corresponding to minimum interior truncation error is within 10% of the value $\alpha = 1.2$ for the sinusoidal exact solution under consideration. The optimal jump coefficient to minimize the boundary truncation error is within the 10% of the value $\alpha = 1.75$. This difference in optimal jump coefficients in interior and boundary regions along with the intuition of using multiple variables to reduce truncation error, as evident from the Equation 4.12, is the motivation for experimenting with two dedicated jump coefficients, each for the boundary and interior edges of the control volumes. Since the truncation error metrics are by definition independent of the solution used, it was also verified that they are not affected by changing the exact solutions tested.

Referring the Equation 4.13, in the absence of a boundary jump term, the error
4.2. Numerical Test Analysis

(a) Interior truncation error

(b) Boundary truncation error

Figure 4.8: Plot for truncation error using single jump term method
4.2. Numerical Test Analysis

Figure 4.9: Case 1: Solution error plot using single jump term method

metric for each control volume is parabolic with respect to the jump coefficient $\alpha$. This behavior is observed globally for the mesh as evident from the parabolic nature of the plots for boundary and interior truncation error. Using the single jump term method, the discretization error for the sinusoidal exact solution is presented in the Figure 4.9. The spike near the jump coefficient $\alpha = 0$ is related to the steep drop in error when a jump term is used. It can also be observed that the solution error minimum has a consistent behavior and that the minimum occurs in the vicinity of the optimal jump coefficient $\alpha = 1.2$, consistent with the truncation error results.

Since truncation error metrics are independent of the problem solved for, the trend for reducing truncation errors with the variation in jump term is the same for exact solution cases 2 and 3. Figures 4.10 and 4.11 show the results for discretization error with a single jump term for cases 2 and 3 respectively. The spike near $\alpha = 0$ shows that SBC has higher errors and the reduction obtained by using single jump term is about two orders of magnitude. The jump coefficient corresponding to the minimum for both the cases are within 20% of the optimal jump coefficient $\alpha = 1.2$ for case 1. Nevertheless, the use of single jump term method is effective for the test cases with regards to truncation and discretization error. It also gives consistent results across the mesh sequence and exact solution cases, as expected from analytic tests.
4.2. Numerical Test Analysis

Figure 4.10: Case 2: Solution error plot using single jump term method

Figure 4.11: Case 3: Solution error plot using single jump term method
4.2. Numerical Test Analysis

Figure 4.12: Comparison of truncation error for different schemes

(a) Interior truncation error

(b) Boundary truncation error
4.2. Numerical Test Analysis

The two jump term implementation is now tested and the results for truncation error is presented in comparison to all the other schemes in the Figure 4.12. Truncation errors for WBC seem to be smaller than SBC but the former case doesn’t yield a converged solution. The Green-Gauss method is shown for the purpose of comparison and as such, it doesn’t give the least truncation error for the boundary. When compared with the use of a single jump term method, the two jump term implementation has half the error magnitude. Thus the two jump term implementation has the least boundary truncation error followed by single jump term method, GGC and then SBC. Interior truncation error is not influenced by the boundary jump term and has the lowest truncation error using the single jump term method followed by SBC and GGC methods. The order of convergence for truncation error is observed to be zeroth.

Figure 4.13 gives an insight as to how the schemes compare when solution error is concerned. All the schemes have a consistent second order rate of convergence as evident from the plot. Using least-squares method with SBC alone has the worst discretization error when compared with the corrected Green-Gauss method and the use of jump terms. The use of single and two jump term methods does not show a greater disparity in solution error since the effect of the boundary jump term is local and limited to the boundary control volumes. Hence we can say with certain surety that the use of two jump terms can potentially reduce the discretization and truncation error. The important factor though is whether all the three measures
4.2. Numerical Test Analysis

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Interior TE Error</th>
<th>α</th>
<th>Boundary TE Error</th>
<th>α</th>
<th>α_B</th>
<th>Discretization Error Error</th>
<th>α</th>
<th>α_B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sq15</td>
<td>0.0554</td>
<td>1.09</td>
<td>0.0225</td>
<td>1.54</td>
<td>1.28</td>
<td>1.27e-03</td>
<td>1.21</td>
<td>2.24</td>
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<tr>
<td>Sq30</td>
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<td>0.0192</td>
<td>1.6</td>
<td>1.34</td>
<td>2.90e-04</td>
<td>1.24</td>
<td>1.25</td>
</tr>
<tr>
<td>Sq60</td>
<td>0.0772</td>
<td>1.18</td>
<td>0.0200</td>
<td>1.57</td>
<td>1.34</td>
<td>7.49e-05</td>
<td>1.21</td>
<td>1.28</td>
</tr>
<tr>
<td>Sq120</td>
<td>0.0746</td>
<td>1.18</td>
<td>0.0199</td>
<td>1.57</td>
<td>1.34</td>
<td>1.81e-05</td>
<td>1.18</td>
<td>2.96</td>
</tr>
</tbody>
</table>

Table 4.6: Optimal jump coefficients for minimum truncation and discretization error

of error have a minimum at same jump coefficients or not. Table 4.6 gives the corresponding jump coefficients associated with the error minima for interior and boundary truncation error and discretization error. We can notice that the minima for interior truncation error and discretization error occur in the close vicinity of $\alpha = 1.2$ but the boundary truncation error minimum occurs in the neighborhood of $\{\alpha = 1.57, \alpha_B = 1.34\}$. The discretization error corresponding to $\alpha = 1.57$ is four times the minimum error achievable and in most cases holds the priority.

Figures 4.16 and 4.17 explain the difference in error distribution for a Sq30 mesh corresponding to cases with minimum for boundary truncation error and discretization error and encourage us to find a trade-off for reducing both the error metrics simultaneously. The variation in boundary truncation error is gradual with the change in jump coefficients. On the other hand, the discretization error changes rapidly with change in jump coefficients and in general is four times the minimum discretization error possible when we use jump coefficients corresponding to minimum boundary truncation error case. The boundary truncation error is also found to be at least two times higher than the minimum possible error when discretization error is minimized.

To select the jump coefficients where both the boundary and discretization error are minimized, we use a Pareto plot for each of the mesh and exact solution combination. Each point on a Pareto plot corresponds to the normalized values of boundary truncation and discretization error for the discrete jump coefficient set on the two jump term space. The boundary truncation error and discretization error are normalized by their corresponding minimum error obtained using the single jump term method. The Pareto plot for a Sq30 mesh for case 1 exact solution is shown in the Figure 4.14, where the points closer to the origin are considered suitable for minimizing both discretization and boundary truncation errors simultaneously. The point with jump coefficients $\alpha = 1.24$ and $\alpha_B = 1.11$ seems to have discretization error and interior truncation error within 1% of their minimum possible values whereas boundary truncation error was within 8% of the minimum, thus achieving.
4.2. Numerical Test Analysis

simultaneous reduction of both the types of errors. The error distribution corres-
ponding to these jump coefficients is also presented in the Figures 4.16 and 4.17
as Optimal error cases.

The interior truncation error hardly varies with boundary jump coefficient as
clearly visible in the Figure 4.18a. Figure 4.18b reveals the behavior of boundary
truncation error with the jump coefficients and we can see that there is a region of
gradual change near the bottom of the surface which spans a significant area in the
α and α_B space. This implies that boundary truncation error can be lowered over
a wider range of jump coefficients. The variation of discretization error in Figure
4.19 also has a flatter surface near the line α = 1.2 and has a range of values
for jump coefficient α_B where it stays in the vicinity of the global minimum for
discretization error. This behavior for all the three measures of error is found to be
the similar across the mesh sequence.

The error distribution for case-2 and case-3 are presented in the Figures 4.20
and 4.21 respectively. We can identify regions where the variation in discretization
error is gradual and it is the overlap of this region with the region for minimum
boundary truncation error that we seek. We find that such regions of minimum er-
rors match for different meshes and different cases of exact solution. This result is
presented in the Figure 4.15 where the deviation of boundary truncation error and
discretization error from their minimum possible error in the two-jump coefficient
space is given for the jump coefficient set {α = 1.24, α_B = 1.11}. Irrespective
of where the minimum for either of the errors occur, the deviation from their min-
imum is less than 30% for discretization error and 10% for boundary truncation
error. The interior truncation error deviates by less than 10% for the jump coeffi-
cient set chosen.
4.2. Numerical Test Analysis

Figure 4.14: Pareto plot for discretization and truncation errors corresponding to case-1 exact solution, Sq30 mesh

Figure 4.15: Pareto case error deviation from minimum possible errors
4.2. Numerical Test Analysis

(a) Minimum boundary TE  (b) Minimum discretization error  (c) Optimal error case

Figure 4.16: Comparison of truncation errors for different minimization cases, Sq30 mesh

(a) Minimum boundary TE  (b) Minimum discretization error  (c) Optimal error case

Figure 4.17: Comparison of discretization errors for different minimization cases, Sq30 mesh
4.2. Numerical Test Analysis

(a) Interior truncation error

(b) Boundary truncation error

Figure 4.18: Truncation error contour plot variation with two jump terms, Sq30 mesh
4.2. Numerical Test Analysis

Figure 4.19: Case 1: Discretization error contour plot using two jump term method, Sq30 mesh

Figure 4.20: Case 2: Discretization error contour plot using two jump term method, Sq60 mesh
4.2. Numerical Test Analysis

4.2.2 Stretched Boundary Layer Mesh

As mentioned in the Chapter 1, the use of stretched grids in the boundary regions is common for viscous flows. The viscous regions require high aspect ratio grid cells and the ways to achieving this condition is by either generating 90 degree triangles or rectangles near the boundary [7, 38, 42]. The behavior of discretization schemes and boundary treatment methods on stretched grids is crucial to understand, for them to be applicable to wider scenarios of flow problems. To generate stretched triangular boundary layered mesh, first a quad layered boundary mesh is constructed around the isotropic triangular square mesh sequence described in the previous section. These quad layers form the new boundary enclosing the triangular mesh as they grow from an aspect ratio of two at the boundary to an aspect ratio of one in the interior. This transition takes place at the growth rate of 1.2 and five quad layers are required (see Figure 5.22 in Section 5.2.2). To generate our stretched boundary layer with triangular elements, these quad elements are randomly split and they acquire the same aspect ratio and growth rates as that of the stretched quad layered mesh. Note that the stretched quad layered mesh is used for numerical tests in Section 5.2.2 and complements the results in this section. Figure 4.22 shows the intermediate meshes in the sequence with a growth layer visible in the boundary. The mesh nomenclature for stretched meshes is Sq#-Str where...
4.2. Numerical Test Analysis

(a) Sq30-Str mesh with 1730 vertices  
(b) Sq60-Str mesh with 5117 vertices

Figure 4.22: Stretched boundary layered triangular mesh

The # corresponds to the original triangular mesh which is modified to include the stretched boundary layer.

The truncation error variation using least-squares reconstruction with strong boundary condition is presented in the Figure 4.23. There is a remarkable similarity in the distribution of errors when compared to the isotropic triangular mesh; however, the magnitude of errors are twice as large as they were for isotropic meshes. Truncation error is maximum in the boundary regions, as expected.

The use of single jump term method has shown considerable deviation with regards to truncation errors. Figure 4.24 gives the variation of interior and boundary truncation error when single jump coefficient is used. The optimal jump coefficient for interior truncation error is $\alpha = 1.0$ whereas that for the boundary truncation error is $\alpha = 2.0$. These jump coefficients are very distinct from each other and different from the jump coefficients observed for the isotropic triangular mesh by at least 20%. Using single jump term method, the discretization errors behave similar to the isotropic mesh cases such that the deviation in jump coefficients is less than 10% compared to the isotropic mesh cases. It is worthwhile to note that the interior truncation errors are higher for stretched meshes compared to isotropic meshes.

The comparison of different schemes for discretization and boundary truncation errors are presented in the Figure 4.25. The results for the two jump term scheme reveal that the truncation errors are lowest for this scheme. They also follow the trend observed for isotropic meshes and are five times smaller than the case where simple SBC scheme is used for boundary treatment. Although the Green-
4.2. Numerical Test Analysis

(a) Error in second derivative of x

(b) Error in second derivative of y

Figure 4.23: Truncation error distribution for Sq30 stretched mesh using least-squares method

Gauss method has lower error compared to a single jump term method, the implementation of boundary condition enforces a flux such that control volume average matches the boundary solution. Hence, the magnitude of boundary truncation error is because of the flux enforcement rather than the Green-Gauss reconstruction method.

Figure 4.25b shows the comparison and convergence of different schemes for discretization error. The convergence is second order accurate and the results are similar to the isotropic mesh cases with the exception of the least-squares method with SBC when linear interpolation is used for face gradient calculation. The mesh Sq120-Str does not yield a converged solution when linear interpolation is used for face gradient calculation. However, the use of arithmetic averaging yields a converged solution. Using jump coefficients also yielded converged solution with the least-squares method when linear interpolation is used and the instability can be attributed to the nature of boundary layers. The discretization errors are lowest for single and two jump term schemes.

Table 4.7 presents the optimal jump coefficients for interior and boundary truncation error as well as for discretization errors. The jump coefficients for boundary truncation errors are vastly different from the results for isotropic meshes. However, they show a consistent pattern across the mesh sequence. Applying the same procedure as for isotropic meshes, a Pareto plot is used to identify points in the two jump coefficient space where the truncation and discretization errors can be simultaneously reduced. The jump term coefficient set of \( \{ \alpha = 1.24, \alpha_B = 0.84 \} \)
4.2. Numerical Test Analysis

(a) Interior truncation error

![Plot for interior truncation error using single jump term](image)

(b) Boundary truncation error

![Plot for boundary truncation error using single jump term](image)

Figure 4.24: Truncation error variation using single jump term for triangular meshes with stretched boundary layers
4.2. Numerical Test Analysis

(a) Boundary truncation error

(b) Discretization error

Figure 4.25: Comparison of different schemes with regards to truncation and discretization error
4.2. Numerical Test Analysis

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Interior TE</th>
<th>Boundary TE</th>
<th>Discretization Error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Error</td>
<td>α</td>
<td>Error</td>
</tr>
<tr>
<td>Sq15_Str</td>
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<td>1</td>
<td>0.4413</td>
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<tr>
<td>Sq30_Str</td>
<td>0.1023</td>
<td>1</td>
<td>0.4465</td>
</tr>
<tr>
<td>Sq60_Str</td>
<td>0.0993</td>
<td>1</td>
<td>0.4648</td>
</tr>
<tr>
<td>Sq120_Str</td>
<td>0.0941</td>
<td>1.03</td>
<td>0.4290</td>
</tr>
</tbody>
</table>

Table 4.7: Optimal jump coefficients for minimum truncation and discretization error, using case 1 exact solution

Figure 4.26: Pareto case error deviation from minimum possible errors

is observed to reduce truncation and discretization error consistently, across different meshes and different exact solution cases. The deviation of discretization and boundary truncation errors for the proposed jump coefficient set from the minimum possible errors for corresponding meshes and exact solution cases is presented in the Figure 4.26. The figure reveals that deviation of errors is less than 10% for boundary truncation error and less than 65% for discretization errors when the proposed jump coefficients are used. The interior truncation errors are well within 10% of their minimum values. Given that the boundary truncation error drops by five times compared to the use of SBC alone and that the discretization error drops by 90% compared to SBC scheme, these deviations seem like reasonable trade-offs.
Chapter 5

Mixed Mesh Results

A triangular mesh near a boundary is sometimes inefficient to capture the boundary information for cases where the mesh is required to be aligned, for example in the direction of flow near a wall. A quad boundary layer can however be aligned with the flow quantities and is expected to have better accuracy compared to a triangular mesh. A purely triangular mesh can be modified to have a quad boundary layer which is an effective and time saving alternative to having a pure quad mesh for complicated geometries, hence generating a mixed mesh. In this chapter, we explore the use of mixed mesh with quad cells at the boundary and triangular cells in the interior with the objective to reduce boundary truncation error while simultaneously achieving accurate solution for a simple diffusion problem. We limit ourselves to studying the effect of quad boundary layers for a diffusion problem leaving the effects on advection for future study.

We proceed as before by using a linear algebra system to analytically evaluate the truncation error in the flux integral for boundary, interior and also the interface control volumes. We employ the schemes used for a purely triangular mesh on a mixed cell mesh and the ones with better reduction in truncation errors are taken forward to implement in the numerical solver ANSLib. As with the triangular mesh results, schemes performing better for the triangular mesh are expected to have similar performance for mixed cells as well. Figure 3.3 shows the mesh used for analytic tests. The square mesh sequence used for triangular tests are modified to have two and five quad boundary layers for numerical tests. The two quad boundary layer mesh is used to study the effect of boundary condition on the interface layer whereas for a five quad layered boundary mesh, the interface layer is in the interior. The following sections present the results for analytic and numerical tests.

5.1 Analytic Test Analysis

This section presents a comprehensive analysis of the schemes for mixed cells. Control volume $i = 25$ represents an interior control volume in Figure 3.3 whereas $i = 40$ is a boundary control volume. The interface control volume is indexed as
5.1. Analytic Test Analysis

The uniform mixed mesh is perturbed in the same way as the triangular
mesh was perturbed, as described in Section 4.1 and summarized in the Figure 4.1
for the five different distortions performed on the mesh. The following sections
scrutinize gradient accuracy and flux integral accuracy followed by the effect of
boundary treatment methods.

5.1.1 Reconstruction Accuracy

The reconstruction accuracy for quad cells in the interior, boundary and interface
control volumes is expected to be first order for both the corrected Green-Gauss
method and the least-squares method. The gradients calculated from either meth-
ods take the form of a linear combination of control volume averages in the stencil
of \( i \). Following the exact same procedure as for the triangular mesh, the control vol-
ume averages in the gradient calculations are expressed as a Taylor series expansion
about the reference control volume to compare the accuracies. The gradient form
for a typical uniform boundary and interface control volume, using least-squares
method are given here.

\[
\hat{\nabla} \phi_{40} = \begin{pmatrix}
\hat{\frac{\partial \phi}{\partial x}} \\
\hat{\frac{\partial \phi}{\partial y}}
\end{pmatrix}_{40} = \begin{pmatrix}
\frac{1}{3}\bar{\phi}_{41} - \bar{\phi}_{39} \\
\frac{1}{3}\bar{\phi}_{35} - \bar{\phi}_{40}
\end{pmatrix} + \frac{1}{4} \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_{40} h + O\left(h^2\right)
\]

\[
\hat{\nabla} \phi_{10} = \begin{pmatrix}
\hat{\frac{\partial \phi}{\partial x}} \\
\hat{\frac{\partial \phi}{\partial y}}
\end{pmatrix}_{10} = \begin{pmatrix}
-0.4\bar{\phi}_9 - 0.2\bar{\phi}_5 + 0.4\bar{\phi}_{11} + 0.2\bar{\phi}_6 \\
0.352(\bar{\phi}_5 + \bar{\phi}_6) - 0.323\bar{\phi}_{10} - 0.381\bar{\phi}_{15}
\end{pmatrix} + \frac{1}{3} \frac{\partial^2 \phi}{\partial x \partial y} \bigg|_{10} h + O\left(h^2\right)
\]

Equation 5.1 gives the discrete gradient for a boundary control volume calcu-
lated using least-squares for the perfect mesh whereas Equation 5.2 gives the gra-
dient for an interface control volume. The discrete gradient is then subtracted from
the exact gradient for an arbitrary control volume, which is given by the Equation 4.3. The general form of the error in gradient is the same as in Section 4.1.1 and presented here for first order gradients.

\[
\tilde{\nabla} \phi_i - \nabla \phi_i = \left( \begin{array}{c} \frac{\partial^2 \phi}{\partial x^2} |_{i} \xi_{xx} + \frac{\partial^2 \phi}{\partial x \partial y} |_{i} \xi_{xy} + \frac{\partial^2 \phi}{\partial y^2} |_{i} \xi_{yy} \h + O(h^2) \\ \frac{\partial^2 \phi}{\partial x^2} |_{i} \eta_{xx} + \frac{\partial^2 \phi}{\partial x \partial y} |_{i} \eta_{xy} + \frac{\partial^2 \phi}{\partial y^2} |_{i} \eta_{yy} \h + O(h^2) \end{array} \right) \tag{5.3}
\]

The Tables 5.1, 5.2 and 5.3 give the gradient error coefficients for boundary, interior and interface control volumes for least-squares and corrected Green-Gauss method. The Green-Gauss method without correction has the same behavior on quad cells as the triangular cells, giving a zero-order gradient for all the three types of control volumes presented. Except for uniform interior quad cells, the order of gradient is zero for uniform or random mesh for all types of control volumes. The gradient errors for least-squares method are again higher in the normal direction compared to the tangential direction. The error for corrected Green-Gauss method is higher than least-squares method in general, a confirmation of the results observed for the triangular test mesh. The error coefficients for the gradients of interface control volumes are comparable to interior control volumes. Hence we can expect the truncation error for interface control volumes to be similar to that of an interior one. It also proves that the least-squares and Green-Gauss method are effective in calculating the gradients at the interface layer without producing significant errors.

### 5.1.2 Flux Integral Accuracy

Table 5.4 gives the order of error in the flux integral which is calculated using the method described in Section 3.1 for boundary, interior and interface control volumes. The results for the least-squares method (LSM) are identical for both arithmetic averaging and linear interpolation methods. The order of truncation for corrected Green-Gauss method is consistent with the expected zero order accuracy for general cases. Without correction, the Green-Gauss method gives one order less accurate flux integral for random and curved meshes, consistent with the observations for a triangular mesh. Since the order of flux integrals for a random mesh is zero, the error metric used for comparing the boundary treatment methods is the same as the one used for triangular mesh.
5.1. Analytic Test Analysis

(a) Error coefficients of $\frac{\partial \phi}{\partial x}$

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\xi_{xx}$</th>
<th>$\xi_{xy}$</th>
<th>$\xi_{yy}$</th>
</tr>
</thead>
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<tr>
<td>Least-Squares</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Random</td>
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<td>$-0.01514$</td>
<td>$-0.00620$</td>
</tr>
<tr>
<td>Green-Gauss Corrected</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<td>0.37500</td>
<td>0</td>
</tr>
<tr>
<td>Random</td>
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<td>0.39745</td>
<td>$-0.00631$</td>
</tr>
</tbody>
</table>

(b) Error coefficients of $\frac{\partial \phi}{\partial y}$

<table>
<thead>
<tr>
<th>Mesh</th>
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<th>$\eta_{xy}$</th>
<th>$\eta_{yy}$</th>
</tr>
</thead>
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<tr>
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</tr>
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<td>Random</td>
<td>0.00732</td>
<td>$-0.47419$</td>
<td>0.43092</td>
</tr>
</tbody>
</table>

Table 5.1: Gradient error coefficients for boundary control volumes

(a) Error coefficients of $\frac{\partial \phi}{\partial x}$

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\xi_{xx}$</th>
<th>$\xi_{xy}$</th>
<th>$\xi_{yy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Least-Squares</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Random</td>
<td>0.21196</td>
<td>0.00479</td>
<td>$-0.00307$</td>
</tr>
<tr>
<td>Green-Gauss Corrected</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>$-0.5$</td>
<td>0.5</td>
<td>0</td>
</tr>
<tr>
<td>Random</td>
<td>$-0.50646$</td>
<td>0.50200</td>
<td>0.00234</td>
</tr>
</tbody>
</table>

(b) Error coefficients of $\frac{\partial \phi}{\partial y}$

<table>
<thead>
<tr>
<th>Mesh</th>
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<th>$\eta_{xy}$</th>
<th>$\eta_{yy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Least-Squares</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Random</td>
<td>$-0.00128$</td>
<td>$-0.02412$</td>
<td>$-0.30029$</td>
</tr>
<tr>
<td>Green-Gauss Corrected</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<td>$-0.5$</td>
<td>0.5</td>
</tr>
<tr>
<td>Random</td>
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<td>$-0.50026$</td>
<td>0.50071</td>
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</tbody>
</table>

Table 5.2: Gradient error coefficients for interior control volumes
5.1. Analytic Test Analysis

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\xi_{xx}$</th>
<th>$\xi_{xy}$</th>
<th>$\xi_{yy}$</th>
</tr>
</thead>
<tbody>
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<td>Least-Squares</td>
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<td>0.17916</td>
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<tr>
<td>Random</td>
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<td>0.11940</td>
<td>−0.00992</td>
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<tr>
<td>Green-Gauss Corrected</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<td>0</td>
<td>0</td>
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<tr>
<td>Random</td>
<td>−0.50446</td>
<td>0.03520</td>
<td>0.02191</td>
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</table>

(a) Error coefficients of $\frac{\partial \phi}{\partial x}$

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\eta_{xx}$</th>
<th>$\eta_{xy}$</th>
<th>$\eta_{yy}$</th>
</tr>
</thead>
<tbody>
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<td>0</td>
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<td>Random</td>
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<td>−0.19762</td>
</tr>
<tr>
<td>Green-Gauss Corrected</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Uniform</td>
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<td>−0.5</td>
<td>0.44424</td>
</tr>
<tr>
<td>Random</td>
<td>−0.14255</td>
<td>−0.42280</td>
<td>0.46126</td>
</tr>
</tbody>
</table>

(b) Error coefficients of $\frac{\partial \phi}{\partial y}$

Table 5.3: Gradient error coefficients for interface control volumes

The order of truncation errors are in agreement with the results of Diskin and Thomas [9]. It should also be noted that a negative order of convergence for truncation error doesn’t necessarily mean a lack of convergence in solution. However, the quad elements have a truncation error which is decoupled and results in solution divergence. Using jump terms has been observed to alleviate this problem, which means using the reconstruction methods alone will not be able to achieve a converged solution. We also implement the gradient correction described by Haselbacher and Blazek [15] and Diskin and Thomas [9] to obtain strongly coupled stencils for both least-squares and Green-Gauss method. This method is presented in the Section 2.2.1 for the Green-Gauss method and the same correction is applied for the least-squares method as well.

Using a jump coefficient of $\alpha = 1$ gives the same exact results for flux integral as it gives with gradient correction for least-squares method on a uniform mesh. However, this behavior deviates for random meshes. The gradient correction replaces the gradient along the edge direction of the two control volumes with an edge derivative whereas a jump term introduces a damping effect to reduce errors. For instance, referring to Section 2.2.1, and defining the directions $\hat{e}$ along the edge of [0,2] and $\hat{n}$ normal to the edge in Figure 2.2 and replacing the gradient on the edge AB with face gradient $\nabla \phi_{02}$, the gradient correction used for both
5.1. Analytic Test Analysis

Table 5.4: Truncation error order comparison for flux integral

\[
\nabla \phi_{AB} = \nabla \phi_{02} + \left[ \frac{\phi_2 - \phi_0}{|r_2 - r_0|} - (\nabla \phi_{02} \cdot \hat{e}) \right] \hat{e} \quad (5.4)
\]

Without the gradient correction, \( \nabla \phi_{02} \) would be the gradient on the edge \( AB \) calculated either through gradient averaging scheme for least-squares or the gradient for the primal cell using the Green-Gauss method. However, to obtain a compact stencil, we can use the correction for the gradient for every edge. To illustrate the effects better, we decompose the gradient \( \nabla \phi_{02} \) into the edge and edge normal direction as shown in Equation 5.5 and substitute in the above equation to see the effect of the gradient correction.

\[
\nabla \phi_{02} = (\nabla \phi_{02} \cdot \hat{e}) \hat{e} + (\nabla \phi_{02} \cdot \hat{n}) \hat{n} \quad (5.5)
\]

\[
\nabla \phi_{AB} = (\nabla \phi_{02} \cdot \hat{n}) \hat{n} + \left[ \frac{\phi_2 - \phi_0}{|r_2 - r_0|} \right] \hat{e} \quad (5.6)
\]

Thus the gradient along the edge direction is replaced by an edge-derivative and the normal component of the gradient is unchanged, which is shown to result
5.1. Analytic Test Analysis

Figure 5.1: Gradient error metrics for different schemes

in a strong coupling. The flux integral without gradient correction for an interior control volume \( i = 25 \) in Figure 3.3 is comprised of second neighbors, as shown in the equation below:

\[
\tilde{\nabla}^2 \phi_i = \frac{1}{4h^2} (\phi_{23} + \phi_{27} + \phi_{35} + \phi_{15} - 4\phi_{25})
\] (5.7)

whereas the flux integral with gradient correction is comprised of immediate neighbors, thus resulting in a compact stencil as shown:

\[
\tilde{\nabla}^2 \phi_{i-GC} = \frac{1}{h^2} (\phi_{24} + \phi_{26} + \phi_{30} + \phi_{20} - 4\phi_{25})
\] (5.8)

A similar effect is also seen for triangular mesh, though the solution is stable even without the gradient correction.

5.1.3 Boundary Treatment Methods

The schemes tested for triangular mesh analysis are applied for quad meshes to verify their consistency. The schemes intended to improve gradient accuracy are the SBC, 4-Unknown and increased stencil size methods. These schemes are tested and compared in reference to the WBC method. The effect of stencil change is shown for all three methods in Figure 5.1 where using increased stencil has higher error metrics compared to a stencil choice of first neighbors. Also, the error in the gradients is minimum for 4-Unknown scheme for the normal gradient followed by SBC and then WBC.
Jump terms can also achieve improved truncation error as observed for the uniform triangular mesh. For a uniform quadrilateral mesh, using jump terms yield a truncation error of the form given in the Equation 5.9. However, there is no gain in accuracy for an interface control volume by using a single jump term method and the order of error remains zero. This is not the case at the boundary, however, where the quadrilateral control volumes allow for a cancellation in error in the tangential direction, leading to a truncation error of the form given in Equation 5.10.

\[
\hat{\nabla}^2 \phi_{\text{int}} - \hat{\nabla}^2 \phi_{\text{int}} = \frac{h^2}{4} \left( \frac{4}{3} - \alpha \right) \left( \frac{\partial^4 \phi}{\partial x^4} \right) + O(h^4) \quad (5.9)
\]

\[
\hat{\nabla}^2 \phi_{\text{bdry}} - \hat{\nabla}^2 \phi_{\text{bdry}} = \frac{7(1 - \alpha)}{15} \frac{\partial^2 \phi}{\partial y^2} + O(h) \quad (5.10)
\]

The optimal jump coefficient for a uniform interior quadrilateral control volume is \( \alpha = \frac{4}{3} \), the same value observed in uniform triangular mesh results and by Nishikawa [30], to yield higher order truncation error. The optimal coefficient for the boundary control volume, however, is \( \alpha = 1 \). The search for an optimal jump coefficient for random meshes using single or two jump terms to gain higher order truncation error was not fruitful. However, the observed jump coefficients are contrasted with the optimal jump coefficients to observe for any similarity.

The different boundary treatment methods are now compared for their performance in reducing truncation error and Figure 5.2 presents the results for a fixed random perturbation of the uniform mesh with weak boundary condition as a reference scheme. SBC, single jump term and two jump term method perform much better than increasing the stencil size or 4-Unknown model. Using gradient correction with SBC have truncation errors comparable to the case where just the SBC scheme is used. Hence we continue with the schemes which are performing well for the boundary truncation error which include single and two jump term methods.

We can also explore the influence of using single jump term method and two jump term method when the quad layers are stretched and randomized simultaneously. This analysis is performed in two ways: one by stretching a random mesh and the other by increasing the randomness of a stretched mesh. The random mesh, generated by perturbing coordinates of a uniform mesh by a maximum of 10% of the edge length, is stretched increasingly from stretch ratios of 0.75 to 1.5. The randomness of a stretched mesh with a stretch ratio of 1.2, is increased by perturbing coordinates proportional to a certain percentage of their edge length. The results
5.2. Numerical Test Analysis

The results observed for analytic tests on a mixed mesh have been consistent with the results observed for a triangular mesh, especially when it comes to proving that using a second jump coefficient gives an extra control variable to reduce the errors, both in truncation and discretization. It has been also pointed out that for a mixed mesh, we encounter the problem of decoupling which results in lack of solution convergence. We use the exact solutions given in Table 4.5 which satisfy the Poisson’s equation with a suitable source term for numerical tests. The use of exact solutions simplifies discretization error calculation; the truncation error

presented in the Figure 5.3 reveal that the two jump term scheme is consistently better at reducing boundary truncation error compared to other methods.

The truncation error for interior and interface control volumes are also compared in Figure 5.4 to see if the effect of having mixed cells produces abrupt increase in error in the interior domain. The errors for interface control volumes compared to interior control volumes are higher for the least-squares method and the single jump term method whereas they are lower for the corrected Green-Gauss method. But when contrasted with the boundary truncation error in Figure 5.2 for the reference scheme of WBC, the errors for both the control volume types are significantly lower. Hence it can be concluded that the reconstruction schemes are effective in calculating the gradients efficiently for the interface layers and thus they can be omitted from the regions of concern for lowering truncation errors.

5.2 Numerical Test Analysis

The results observed for analytic tests on a mixed mesh have been consistent with the results observed for a triangular mesh, especially when it comes to proving that using a second jump coefficient gives an extra control variable to reduce the errors, both in truncation and discretization. It has been also pointed out that for a mixed mesh, we encounter the problem of decoupling which results in lack of solution convergence. We use the exact solutions given in Table 4.5 which satisfy the Poisson’s equation with a suitable source term for numerical tests. The use of exact solutions simplifies discretization error calculation; the truncation error
5.2. Numerical Test Analysis

(a) Increasing stretch ratio for random mesh

(b) Increasing randomness of a stretched mesh

Figure 5.3: Comparison of single and two jump term methods on randomly stretched meshes

Figure 5.4: Comparison of interior and interface truncation errors
metrics are calculated as explained in Section 3.2.1 and are independent of the exact solution used but depend on the mesh.

5.2.1 Isotropic Boundary Layer Mesh

We continue to use a unit square domain for our numerical tests; however the triangular mesh is modified to include quad boundary layers. Each of the triangular square meshes used for numerical tests in the previous chapter now has two and five isotropic quad layers added at the boundary, resulting in two different sequences of meshes. The mesh is scaled such that the domain is a unit square and has the same triangular mesh in the interior with the quad layers grown near the boundary. The mesh is of high quality with gradual change in size and is presented in the Figure 5.5. The square mesh with five isotropic quad layers is used primarily to analyze the schemes to reduce truncation error whereas the square meshes with two quad layers is used to observe the impact of having an interface layer interact with the boundary control volumes. The interface layer in two quad layered meshes have flux integrals which include the boundary control volume information directly. Finally, we also study a sequence of pure quad meshes which have characteristic length scales comparable with the isotropic pure triangular mesh. They are labeled as Quad-#x# where the number is equal to the square root of the total number of primal cells in the mesh. The nomenclature for the mixed mesh is straightforward.

Truncation error distributions for square meshes with two and five quad boundary layers is presented in the Figures 5.6 and 5.7 respectively. The error distributions observed for second derivatives in the x and y direction reveal that the boundary control volumes and their first neighbors are the regions of maximum error. Hence we continue with our approach of using boundary error metric to account for the truncation error in boundary control volumes and their first neighbors whereas an interior truncation error metric measures the error for the interior control volumes. Some conclusions can be readily made from the figures, which are that the interface layer blends well with the interior for a square mesh with five quad layers. The fact that error distributions for a square mesh with two quad layers are similar to that of a five quad layered mesh with no spikes in the interface layer confirms that a transition from triangular to quad mesh is smooth.
5.2. Numerical Test Analysis

(a) Sq30 mesh with five isotropic quad layers
(b) Sq60 mesh with five isotropic quad layers
(c) Sq30 mesh with two isotropic quad layers
(d) A 32x32 pure quad mesh

Figure 5.5: Isotropic meshes for numerical analysis
5.2. Numerical Test Analysis

(a) Error in second derivative of x  
(b) Error in second derivative of y

Figure 5.6: Truncation error distribution for Sq30 mesh with two isotropic quad layers, using LSM

(a) Error in second derivative of x  
(b) Error in second derivative of y

Figure 5.7: Truncation error distribution for Sq30 mesh with five isotropic quad layers, using LSM

The schemes found analytically to be effective in reducing truncation error for a mixed mesh are the least-squares method with strong boundary condition (SBC) and the single and two jump term methods. The two jump term method uses a weak boundary condition whereas the single jump term method uses a strong boundary condition; both employing least-squares gradient reconstruction. Since the use of least-squares method with SBC alone doesn’t yield a converged solution, the
5.2. Numerical Test Analysis

method is used only for comparison of truncation errors. However, we focus on the use of least-squares method with gradient correction and strong boundary condition (LSM-GC) to compare with other schemes for reduction of error in truncation and discretization. The corrected Green-Gauss method is also presented as an alternative method of solution reconstruction to compare with least-squares method in general.

The convergence of the solution is first verified for all three mesh sequences in Figure 5.8 and for this purpose the least-squares method with gradient correction (LSM-GC) is used to avoid decoupling. We compare the face-gradient averaging methods which include the linear interpolation (LI) and arithmetic averaging (AA) for least-squares method and find that the differences are negligible for discretization errors and the order of convergence is indeed second order with the gradient correction as well. The Green-Gauss method with correction (GGC) and without correction (GG) are also compared for solution convergence. As expected, the normal Green-Gauss method shows a one order lower accuracy in convergence of the errors in control volume averages; this is well remedied by the corrected Green-Gauss method for gradient calculations, showing a second order convergence. The gradient corrected least-squares method has better accuracy when compared to the Green-Gauss method. The errors for pure quad meshes are comparable but lower than the mixed meshes.

Figures 5.9 and 5.10 give the variation of truncation errors using the single jump term method for the mesh sequence with two and five quad layers along with pure quad meshes. It can be observed that the jump coefficient required to minimize the boundary truncation error is starkly different from the jump coefficient required to minimize interior truncation error. The optimal jump coefficient for interior truncation error for the mixed meshes is in the neighborhood of $\alpha = 1$ whereas for the pure quad meshes, it varies little from the optimal coefficient of $\alpha = 0.9$ across the sequence. This is different from the results observed for the interior truncation error obtained for a pure triangular mesh where the optimal jump coefficient was around $\alpha = 1.2$.

The optimal jump coefficients for boundary truncation error metrics is around the value of $\alpha = 1.75$ for both the mixed and pure quad meshes, and it is strikingly closer to the value observed for a pure triangular mesh. However, the parabolic nature of the curve for truncation error metrics, both interior and boundary, with respect to the jump coefficients confirms the results predicted by analytic tests and those observed for triangular meshes. It also implies that the flatter minimum for the curve can accommodate a broader range of jump coefficients to achieve reduced truncation error.

The variation of discretization error for mixed meshes with five quad layers is presented in Figure 5.11. The optimal jump coefficients for a sequence of meshes
5.2. Numerical Test Analysis

(a) Square meshes with five isotropic boundary quad layers

(b) Square meshes with two isotropic boundary quad layers

(c) Pure Quad mesh sequence

Figure 5.8: Convergence of solution using least-squares and Green-Gauss methods
5.2. Numerical Test Analysis

(a) Square meshes with two quad layers

(b) Square meshes with five quad layers

(c) Pure quad meshes

Figure 5.9: Interior truncation error using single jump term
5.2. Numerical Test Analysis

Figure 5.10: Boundary truncation error using single jump term
for a particular case of exact solution is consistent; however, there are variations as the exact solution changes. The optimal jump coefficient varies from the coefficients $\alpha = 0.9$ for logarithmic solutions to $\alpha = 1.2$ for sinusoidal solution. The optimal jump coefficient for non-homogeneous sinusoidal exact solution case is $\alpha = 1$. These results were found to be similar for the mixed mesh sequence with two quad layers as well.

The variation of discretization error for the pure quad mesh sequence is given in Figure 5.12. The optimal jump coefficients are again consistent across the sequence for a particular exact solution but are dissimilar across the cases. The optimal coefficients in comparison with the mixed mesh are very similar for cases 2 and 3 but for case 1, they resemble the optimal jump coefficient for a uniform quadrilateral mesh. The optimal jump coefficient of $\alpha = \frac{4}{3}$ was observed to yield a fourth order truncation error for uniform mesh, as shown by the Equation 5.9 and is also the point where case 1 yields minimum discretization error.

The conclusions for mixed and pure quad meshes are harder to draw as there is a subtle variation in the jump coefficients with the change in exact solutions. However, it should be noted that there is a certain degree of consistency for the optimality of jump coefficients when the mesh is changed in a sequence. The reduction in error by the use of jump coefficients is certainly an effect seen for all the cases of exact solutions and mesh sequences. The drop in error for the exact solutions tested is at least twenty times compared to no-jump term scenarios, across the mesh sequences for triangular, mixed and pure quad meshes.

So far, we have discussed the results for a single jump term method. The other methods under consideration are the use of least-squares method with gradient correction and two jump term method. The results for interior and boundary truncation error using different schemes are compared in the Figures 5.13, 5.14 and 5.15 for mixed two and five quad layered, and pure quad meshes respectively. Interior truncation error is maximum for the case of Green-Gauss method followed by least-squares method without gradient correction (LSM) and with gradient correction (LSM-GC). The use of jump term has considerably lower truncation error as expected. The over all truncation error in the interior is lesser for the quad elements for all the schemes when compared to the mixed meshes.

Near the boundary, the use of jump terms and gradient corrected least-squares method reduces the truncation error drastically when contrasted with the Green-Gauss method or the normal least-squares method. Consistent with the observations for triangular mesh, the use of two jump terms produces the least truncation error near the boundary followed by the gradient corrected least-squares method used to reduce decoupling in the flux integral. The use of gradient correction is similar but not the same as the use of jump terms and hence the lower truncation error when compared to other methods. The magnitudes and behavior for all the
5.2. Numerical Test Analysis

(a) Case 1: Sinusoidal solution, homogeneous boundary condition

(b) Case 2: Logarithmic solution, homogeneous boundary condition

(c) Case 3: Sinusoidal solution, non-homogeneous boundary condition

Figure 5.11: Plot for solution error on square meshes with five boundary quad layers, using the single jump term method
5.2. Numerical Test Analysis

(a) Case 1: Sinusoidal solution, homogeneous boundary condition

(b) Case 2: Logarithmic solution, homogeneous boundary condition

(c) Case 3: Sinusoidal solution, non-homogeneous boundary condition

Figure 5.12: Plot for solution error on pure quad square meshes, using the single jump term method
5.2. Numerical Test Analysis

(a) Interior truncation error

(b) Boundary truncation error

Figure 5.13: Comparison for truncation error on square meshes with two quad layers
5.2. Numerical Test Analysis

(a) Interior truncation error

(b) Boundary truncation error

Figure 5.14: Comparison for truncation error on square meshes with five quad layers
5.2. Numerical Test Analysis

Figure 5.15: Comparison for truncation error on pure quad meshes
three mesh sequences is identical since the boundary layer is basically composed of quadrilateral elements.

A summary of the comparison of schemes with respect to the discretization error is presented in the Figure 5.16. In case of discretization error, the use of jump terms acts as a damping term which alleviates the decoupling issues otherwise observed when the simple least-squares method is used. We observed in triangular mesh results that the use of the least-squares method alone had errors significantly higher than the Green-Gauss method and the jump term methods. For mixed and pure quad meshes, we lack such a comparison as the least-squares fails to converge by itself. This also explains why the use of least-squares method with gradient correction has errors comparable to those observed with the jump term methods. The discretization error continues to be less dependent on the boundary jump coefficient compared to interior jump coefficient and hence the errors are very close for both single and two jump term methods.

The discussion is now focused on exploring the jump coefficients for achieving simultaneous reduction in truncation and discretization errors. Table 5.5 presents the results for the the optimal jump coefficients associated with each of the interior truncation error, boundary truncation error and discretization error. The wide disparity in the jump coefficients required to minimize different aspects of errors can be observed for different mesh sequences. The results for the mixed square mesh sequence with two and five quad layers are very similar with regards to all the three measures of errors. Only the truncation error is minimized in a narrow band of jump coefficients for mixed and pure quad meshes.

The question now remains to find the jump coefficients that simultaneously reduce truncation errors for interior and boundary as well as discretization errors. We aim to keep the optimal scenario errors within 20% of the minimum possible errors for interior and boundary truncation error and the same is anticipated for discretization error. The discretization errors and boundary truncation errors corresponding to each discrete jump coefficient set in the two jump term space are normalized by their respective minimum errors obtained using the single jump term method and are plotted as a Pareto plot. Figure 5.17 shows the Pareto plots for case 1 exact solution on a mixed mesh with five quad layers and a pure quad mesh. The points of interest are the points in the bottom-left corners which are closer to both the axis and are the points of minimum for boundary truncation errors and discretization errors.

This analysis, similar to the isotropic triangular mesh case, is performed for all the exact solution cases and different mesh sequences. A particular point on the jump term space is explored for the mixed mesh and pure quad mesh sequence and the deviation from the minimum errors possible are calculated. Figure 5.18 shows the results for deviation of the errors from minimum possible for the mesh
5.2. Numerical Test Analysis

(a) Square meshes with two isotropic boundary quad layers

(b) Square meshes with five isotropic boundary quad layers

(c) Pure quad mesh sequence

Figure 5.16: Comparison of solution using least-squares and Green-Gauss methods
### Table 5.5: Optimal Jump Coefficients for Minimum Truncation and Discretization Error, Using Case 1 Exact Solution

<table>
<thead>
<tr>
<th>Mesh</th>
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<th>Boundary TE</th>
<th>Discretization Error</th>
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</thead>
<tbody>
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<td>Error</td>
<td>$\alpha$</td>
<td>Error</td>
</tr>
<tr>
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<td>1</td>
<td>0.2029</td>
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<td>Sq30_ISO_2Quad</td>
<td>0.0992</td>
<td>1</td>
<td>0.2019</td>
</tr>
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<td>1</td>
<td>0.2041</td>
</tr>
<tr>
<td>Sq120_ISO_2Quad</td>
<td>0.0931</td>
<td>1.03</td>
<td>0.2017</td>
</tr>
<tr>
<td>Sq15_ISO_5Quad</td>
<td>0.0820</td>
<td>0.94</td>
<td>0.1788</td>
</tr>
<tr>
<td>Sq30_ISO_5Quad</td>
<td>0.0916</td>
<td>0.97</td>
<td>0.1830</td>
</tr>
<tr>
<td>Sq60_ISO_5Quad</td>
<td>0.0923</td>
<td>0.97</td>
<td>0.1797</td>
</tr>
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<td>0.1822</td>
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</tr>
<tr>
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<tr>
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<td>0.88</td>
<td>0.1694</td>
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<td>Quad128x128</td>
<td>0.0595</td>
<td>0.88</td>
<td>0.1642</td>
</tr>
</tbody>
</table>

(a) Square mesh with two quad layers

(b) Square mesh with five quad layers

(c) Pure quad meshes
5.2. Numerical Test Analysis

(a) Sq30 mesh with five quad layers

(b) Quad 32x32 mesh

Figure 5.17: Pareto plot for discretization and boundary truncation error corresponding to case-1 exact solution
sequences and for each of the exact solution cases. The gain in accuracy for boundary truncation error using two jump term method is about eight times the error when simple least-squares method is used. The gain in solution accuracy is about 20 times when jump terms are used compared to the case of none or almost zero jump coefficients. Thus using Pareto plot, we choose points so that boundary truncation errors deviate by a maximum of 20% from their global minimum while the discretization error are kept as close to the global minimum as possible.

The results for the mixed mesh sequence with five quad layers is presented for the jump coefficients \( \{ \alpha = 1.24, \alpha_B = 1.11 \} \) chosen from the Pareto plot whereas for the pure quad mesh sequence we used the jump coefficients \( \{ \alpha = 1.36, \alpha_B = 1.11 \} \). The solution errors for mixed meshes deviate by a maximum of 35% from the minimum possible errors for all exact solution cases. For pure quad meshes, the deviation from the minimum possible error is about 20% for cases 1 and 3 but for case 2, the deviation is about 100%. Despite the variations, the drop in discretization error is at least ten times or more the error for reference case of almost zero jump coefficient, in all the scenarios. The deviation for boundary truncation error for mixed and pure quad meshes is about 20% from the minimum possible errors. The interior truncation error deviates by about 10% for the mixed mesh sequence of two and five quad layers, for the jump coefficients used for Pareto case. The results for mixed meshes with two quad layers follow the results observed for the mixed meshes with five quad layers. The interior truncation error for the pure quad mesh sequence is on the higher side of 20-25% for the jump coefficient of \( \alpha = 1.36 \).

The variation of boundary truncation error using two jump term method for a five quad layered mixed mesh and a pure quad mesh is shown in the Figure 5.19. The contours are similar since the boundary has quad layers for both the meshes. The contours for interior truncation error are parabolic and independent of the variation in the boundary jump coefficient. The variation of discretization errors are also given for the five quad layered mixed mesh and pure quad mesh in the Figures 5.20 and 5.21 respectively. The region for lower errors are concentrated along lines of constant alpha for different cases of exact solutions. There is slight dependence on the boundary jump coefficients for discretization errors.
5.2. Numerical Test Analysis

(a) Square mesh sequence with five quad layers

(b) Pure quad mesh sequence

Figure 5.18: Pareto case error deviation from minimum possible errors
5.2. Numerical Test Analysis

Figure 5.19: Variation of boundary truncation error in two-jump term space

(a) Sq30 mesh with five quad layers

(b) Quad 32x32 mesh
5.2. Numerical Test Analysis

(a) Exact Solution Case 1

(b) Exact Solution Case 2

(c) Exact Solution Case 3

Figure 5.20: Variation of discretization error in two-jump term space for Sq30 mesh with five Quad layers
5.2. Numerical Test Analysis

(a) Exact Solution Case 1

(b) Exact Solution Case 2

(c) Exact Solution Case 3

Figure 5.21: Variation of discretization error in two-jump term space for a 32x32 pure quad mesh
5.2. Numerical Test Analysis

5.2.2 Stretched Boundary Layer Mesh

The meshes tested in the previous section had an isotropic quad boundary layer. Sometimes, a growth in the boundary layer is desired to allow for high aspect ratios closer to the boundary without increasing the cell count drastically. This section discusses the results for such a sequence of meshes where the boundary layer has high aspect ratio cells near the wall which increase in height as they grow towards the interior. Two and five quad layers are grown around the pure triangular mesh sequence with a growth rate of 1.2 to complement the isotropic mixed meshes that have been previously tested. The aspect ratio at the interface layer is maintained as one whereas for five quad layered mesh, the aspect ratio is two for the quads at the boundary. The aspect ratio is 1.25 for the boundary quads in the two quad layered mesh. The meshes are shown in the Figure 5.22 where the growth in the quad layers is moderate but significant enough to differ from the isotropic mesh sequence. The two quad layered mesh doesn’t show a greater deviation from the isotropic mesh but the effect of stretched mesh can be better studied with the mesh sequence of five stretched quad layers.

The distribution of truncation error metrics for a Sq30 mesh with five stretched quad layers is presented in Figure 5.23. The results are very similar to the case of a square mesh with isotropic quad layers when least-squares reconstruction is used. The solution convergence was also found to be second order when the least-squares method with gradient correction or the corrected Green-Gauss method was used.
5.2. Numerical Test Analysis

(a) Error in second derivative of $x$

(b) Error in second derivative of $y$

Figure 5.23: Truncation error distribution for Sq30 mesh with five stretched quad layers using LSM

The normal Green-Gauss method had the same behavior as before, with first order convergence. This trend was the same for both mesh sequences with two and five stretched quad layers.

The variation of interior truncation error with a single jump term was almost identical to the cases where the boundary layer wasn’t stretched. However, an inspection of the boundary truncation error reveals that the optimal jump coefficients for minimum truncation error differs from the isotropic quad layer cases. Figure 5.24 reveals the differences in the results for stretched quad layers. The optimal jump coefficient of $\alpha = 1.75$ for two quad layered meshes is similar to the case of isotropic boundary layered meshes but the optimal jump coefficient for five stretched quad layered meshes is $\alpha = 1.98$. This optimal jump coefficient for five quad layered stretched meshes is the same as the optimal jump coefficient of $\alpha = 2$ for stretched triangular meshes which were in fact derived from the same five quad layered stretched mixed meshes. It is also noted that the truncation errors are marginally higher for stretched meshes.

We compared the boundary truncation error for jump term schemes, gradient corrected least-squares reconstruction and the corrected Green-Gauss method as shown in Figure 5.25. Contrary to our expectations from results for isotropic mesh where the two jump term method had the lowest boundary truncation errors, the use of a single jump term appears to have the lowest truncation error for a stretched mesh with five quad layers. This also contradicts the prediction in the analytic tests where randomly stretched meshes (see Figure 5.3) showed two jump term scheme to be superior to single jump term method in reducing boundary truncation.
5.2. Numerical Test Analysis

(a) Mesh sequence with two stretched quad layers

(b) Mesh sequence with five stretched quad layers

Figure 5.24: Boundary truncation error variation using single jump term method
5.2. Numerical Test Analysis

error. The triangular stretched meshes were consistent with the results observed for isotropic meshes and also had lowest errors for two jump term scheme than any other method. This anomaly in results warrants further inspection especially for stretched quad meshes.

Also presented in the Figure 5.25 are the results for the least-squares method with SBC which is given for the sake of comparison even though the solution doesn’t converge for this scheme. The Green-Gauss method shows a considerably higher truncation error whereas least-squares method with gradient correction has reasonably good accuracy, just after the two jump term method. For a five quad layered sequence, the single jump term method has the lowest error whereas for two quad layered meshes, the errors for the two jump term method are the lowest.

The mixed stretched quad layered meshes have results similar to isotropic mixed meshes when it comes to discretization error and interior truncation errors. The interior truncation errors behave the same way as they did for isotropic quad layered meshes whereas the results for discretization error are given in the Figure 5.26. The two jump term and single jump term method are again the best in reducing the discretization error followed by the gradient correction used for least-squares method.

Since the single jump term method has lower boundary truncation error compared to two jump term scheme, the simultaneous reduction of errors is difficult to be limited to a minimum deviation of 20%. Applying the same procedure used for isotropic boundary layer mesh, jump coefficients are identified in the two jump term space to reduce truncation and discretization errors. The deviation of errors, corresponding to jump coefficient set of \( \{\alpha = 1.24, \alpha_g = 0.84\} \), from the minimum possible errors for boundary truncation and discretization error are presented in the Figure 5.27. The discretization errors deviate by a maximum of 100% from their minimum possible values for all exact solution cases, whereas the boundary truncation error deviates by about 35% from their minimum values achieved using the single jump term method. An alternate approach was to use a single jump term scheme and the best errors were realized at the interior jump coefficient of \( \alpha = 1.4 \). The boundary truncation error deviated by 35% but discretization errors deviate by at least 100-400%. Hence, the two jump term scheme serves as the best scheme in reducing truncation errors and discretization errors simultaneously, across different mesh types. However, prior to making any assumptions about the best approach suited when the boundary has stretched quad layers, it warrants further inspection of results and causes for the behavior of two jump term scheme. Hence, this discussion is left for future studies.
5.2. Numerical Test Analysis

(a) Mesh sequence with two stretched quad layers

(b) Mesh sequence with five stretched quad layers

Figure 5.25: Comparison of boundary truncation error for different schemes on mixed mesh
5.2. Numerical Test Analysis

(a) Mesh sequence with two stretched quad layers

(b) Mesh sequence with five stretched quad layers

Figure 5.26: Comparison of solution error for different schemes on mixed mesh
5.2. Numerical Test Analysis

Figure 5.27: Pareto case error deviation from minimum possible errors
Chapter 6

Summary and Conclusions

6.1 Summary

This thesis presents techniques aimed at reducing the truncation error at the boundary specifically, and the discretization and overall truncation error in general. A finite volume formulation was used to solve the governing equations with a vertex-centered control volume approach for triangular and mixed meshes. The comparison of truncation error was made possible by defining an error metric. This metric was based on the magnitude of coefficients associated with each of the spatial derivatives of the Taylor series expansion of the truncation error for an arbitrary solution. The discretization error was calculated by using the Method of Manufactured Solutions, where a set of three exact solutions were used throughout the thesis for a robust comparison.

The techniques have been discussed for a diffusion problem, using Poisson’s equation as the model. A sequence of triangular, quad, and mixed meshes with quad boundary layers and triangular interiors were considered for analyzing the effects of different schemes developed to reduce truncation and discretization errors. The second order least-squares and the Green-Gauss solution reconstruction methods were described in detail. The subtleties of using the vertex as a reference point instead of the centroid for the control volume were also highlighted for the Green-Gauss methods.

The schemes proposed for reducing error were evaluated systematically using analytical and numerical approaches. The analytical approach gives an algebraic representation for the behavior of schemes with respect to truncation error. It is a direct extension of the Taylor series analysis used for structured meshes. Regular topological meshes, both triangular and mixed, were used for evaluating different schemes for asymptotic order of convergence and magnitude of errors. These tests yield the general form of the truncation error for different scenarios and serve as the first screening process to eliminate schemes which perform poorly for systematically perturbed meshes. The tests were performed on a family of systematically perturbed meshes to make the results applicable for general scenarios.

The use of analytical tests is restricted to regular topological meshes with fixed connectivity and is extended to more general and unstructured meshes through
6.2 Conclusions

The objective of attaining simultaneous reduction of truncation and discretization error for general isotropic and stretched unstructured meshes is accomplished satisfactorily. A wide range of schemes were applied to implement the boundary condition either through improving the solution reconstruction, increasing stencil size, using ghost cells or jump terms as alternate approaches. The following discussion compares and contrasts the analytical and numerical results for the triangular, quad and mixed meshes.

Analytical tests showed the gradients to have lower error when the least-squares method was used in comparison to the Green-Gauss method and also demonstrated that augmenting stencil size was not fruitful beyond a point. It was also shown that strong boundary condition (SBC) and 4-Unknown models (4Unk) have better gradients at the boundary compared to weak boundary condition (WBC) for the least-squares method. It was noted that using vertices as reference points for calculating gradients by the Green-Gauss method yielded zero order gradients and first order solution convergence whereas using centroids as reference points produced the much desired first order gradients and second order convergence for the
6.2. Conclusions

Analytic tests determined that the truncation error for triangular, quad and mixed meshes is at best zeroth order for randomly perturbed meshes in both the interior and boundary regions as well as for interface layers on mixed meshes. The potential of jump terms to increase the effective order of accuracy for truncation errors on uniform meshes was also highlighted. Only the uniform mesh quad boundary layers showed an improvement in accuracy of truncation error by one order for positive jump coefficients; this was not possible for uniform triangular meshes. The interface layer for uniform meshes, although in the interior region, has zero order truncation error accuracy for any discretization scheme. Second order truncation error accuracy was observed only for interior control volumes on uniform, scaled, and sheared meshes across different element types.

The general form of truncation error revealed decoupled flux integrals for quad elements which was remedied by a gradient correction scheme. Both the least-squares and the Green-Gauss methods were prone to decoupling and particularly for least-squares, this led to divergence in numerical tests in the absence of a gradient correction.

Implementation of different boundary treatment methods, including jump term methods and gradient correction schemes, have shown second order convergence for discretization error, across different mesh types and exact solution cases. Using mixed cell meshes, the interface layer was shown to be similar to interior regions with regards to truncation and discretization error. The errors were marginally higher for the interface layer when compared to interior regions with regards to truncation or discretization errors but were much less than the boundary regions.

The face gradient calculation for the least-squares method using arithmetic averaging and linear interpolation showed little difference for discretization or truncation error. The Green-Gauss method had reasonable solution accuracy for triangular, quad and mixed meshes while the truncation errors were higher compared to other schemes for all element types.

The numerical results for all the mesh sequences showed significant reduction in discretization and interior truncation errors using the single and two jump term methods. The Green-Gauss and least-squares methods with SBC and gradient correction when needed were the next best schemes to reduce discretization errors. The boundary truncation error was best minimized when the two jump term method was used for implementing the boundary condition on isotropic meshes. Interior truncation error was independent whereas discretization error was less sensitive to the changes in the value of boundary jump coefficient. Using the single jump term method, the optimal jump coefficients for minimizing the interior and boundary truncation errors had distinct values; discretization error showed slight variation in optimal jump coefficients when the exact solutions were changed, for all the mesh
6.2. Conclusions

Using two jump term method, the set of optimal jump coefficients for reducing each of the interior truncation error, the boundary truncation error and the discretization error are different. However, a Pareto plot enabled us to find a point in the two jump term space such that all the three errors are minimized simultaneously within a certain range of their minimum possible values. On isotropic triangular and mixed meshes, a two jump coefficient set of \( \alpha = 1.24, \alpha_B = 1.11 \) was identified. For this jump coefficient set, the overall truncation and discretization error had a deviation of about 20-30% from their respective minimum possible values across the sequence and for different exact solution cases tested. The jump set of \( \{ \alpha = 1.36, \alpha_B = 1.11 \} \) was also identified for quad meshes but the variation for discretization error was about 100% whereas the truncation error was allowed to deviate by about 20% from their respective minimums.

Thus using two jump term methods, the simultaneous reduction of truncation error and discretization error for an isotropic mesh was made possible in this thesis. When mixed five stretched quad layered meshes were used, the advantage of using two jump terms was lost as the single jump term scheme had the lowest errors. This was in contrast to the results observed for stretched triangular boundary layered meshes, where two jump term scheme consistently resulted in lowest boundary truncation errors. The analytical results for stretched quad layers also pointed at the superior performance of two jump term scheme over single jump term method.

A Pareto plot analysis for stretched five quad layered meshes was performed and the deviation from their minimum possible errors for discretization and boundary truncation errors using the jump coefficient set \( \{ \alpha = 1.24, \alpha_B = 0.84 \} \) were about 100% and 35% respectively. This scenario using two jump term method was better than using the single jump term method to reduce errors simultaneously. A similar analysis for the stretched triangular boundary layered meshes, using the jump coefficient set of \( \{ \alpha = 1.24, \alpha_B = 0.84 \} \) showed a maximum deviation of 65% for discretization errors and about 10% for overall truncation error.

This conclusion proves that the two jump term scheme has successfully reduced truncation and discretization errors for any mesh type or exact solution type tested in this thesis. However, the anomaly in the performance of the two jump term scheme for stretched quad layered boundary meshes warrants further research before any reliable suggestions can be made for the success in this category of meshes.

For the isotropic and stretched mesh families, the truncation errors near the boundary with quad layers were in general lower than in the case of triangular meshes, though the gain was not phenomenal. The interior truncation error for a pure quad domain is only slightly better than that for the pure triangular meshes. This implies that there are no significant gains with regards to diffusion when an
unstructured mesh is used with either triangular or quad boundary layers. Using stretched meshes only increased the truncation error near the boundary.

In conclusion, it is noted that using the two jump term scheme has reduced truncation errors by at least five times for isotropic triangular and mixed meshes as well as quad and stretched triangular meshes when compared to the use of SBC alone. Using the single or two jump term methods has reduced boundary truncation errors by about 2-3 times for stretched five quad layered meshes compared to SBC method. The discretization errors decrease at least by a factor of 10-20 times for all the mesh types using either of the jump term schemes for the exact solutions tested. The interior truncation error was approximately halved by using jump terms compared to the no jump term scenario.

6.3 Recommended Future Work

The techniques and results presented in this thesis have answered most of the questions that were posed at the onset of this research. The techniques developed in this work can be used to reduce different forms of errors simultaneously for isotropic triangular, quad and mixed meshes. However, the scope of research was limited by certain factors and new avenues were identified where the research can be taken forward in order to answer questions that arose during the course of this thesis. The following are considerable ways the research can be extended

1. The control volume averages for ghost cells were extrapolated from the interior regions using a simple second order scheme. Effective ways of extrapolating information to the ghost cells with higher order accuracy is anticipated to give better truncation errors than those observed in this work. It would be interesting to see if this suggestion can lead to truncation errors better than the two jump term method.

2. The boundary treatment methods were tested mostly on isotropic meshes. Performance of these methods on anisotropic meshes is a missing piece to the puzzle in understanding the behavior of truncation and discretization errors.

3. The analysis for the boundary truncation error can be easily extended to cell-centered control volume methods. The inclusion of boundary constraints and jump terms for a cell-centered framework is already available in the literature. The assessment of different schemes on cell centered methods is a considerable study that can be pursued.
6.3. Recommended Future Work

4. The research presented was limited to second order methods and the extension to higher order methods is crucial in understanding the behavior of these schemes. The extension would entail the calculation of higher order flux Jacobians, higher order moments and higher order reconstruction methods.

5. Extension of the current methodology from 2D to 3D versions will be challenging yet necessary if the effect of the schemes on real-life problems are to be understood. 3D reconstruction and 3D Jacobian calculation are reasonably straightforward, however the storage requirements could be an issue of concern.

6. Ultimately, the analysis can be extended from a simple diffusion problem to more general fluid flow phenomena governed by the PDEs such as the Euler or Navier-Stokes equations.
Bibliography


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