Implementation and Validation of a New Spectral Difference Method for Hyperbolic Conservation Laws Using Raviart-Thomas Elements

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A thesis submitted in partial fulfillment for the degree of Master of Science in Simulation Sciences

in the
German Research School for Simulation Sciences
RWTH Aachen University

January 2011
Declaration of Authorship

I, Aravind Balan, hereby declare that I have created this work completely on my own and used no other sources or tools than the ones listed, and that I have marked any citations accordingly.

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Abstract

Numerical schemes using locally discontinuous polynomial approximation are very popular for high order approximation of conservation laws. While the most widely used numerical schemes under this paradigm appears to be the Discontinuous Galerkin method, the Spectral Difference scheme has often been found attractive as well, because of its simplicity in formulation and implementation. Linear stability analysis studies showed that the scheme in its original form is not unconditionally linearly stable for triangular mesh elements. However, recently it has been shown that the scheme is linearly stable for triangles, if we use Raviart-Thomas polynomial space for flux interpolation.

The present thesis work aimed at implementing this new variant of the Spectral Difference scheme in 2-dimensional domains to solve the linear advection equation and also the Euler equations, thereby proving its usability for more complex fluid flow problems. Full order of convergence was achieved for the linear advection problem. The Euler equations were solved around an airfoil for the subsonic flow cases. The flow features were captured well even with a coarse mesh. Linear stability analysis was performed and an optimal Strong Stability Preserving (SSP) time stepping scheme was analyzed with the new Spectral Difference discretization.
First and foremost, I would like to thank my mentor Prof. Georg May for his insightful supervision, guidance and encouragement throughout my work. The several discussions I had with him were inspiring, and I really appreciate his patience. I am indebted to my colleague Francesca for her prompt helpfulness. She used to come to my aid almost immediately whenever I sought her help. I gratefully acknowledge Jochen and Francesca for their time and effort that went into correcting my thesis. Special thanks are due to my office-mates Roman, Matthias and Diego for their several valuable contributions. I consider it an honor to be a part of the research at AICES graduate school, and I appreciate all those who were part of my life here. The financial support from the Deutsche Forschungsgemeinschaft (DFG) through grant GSC 111 is gratefully acknowledged.

Finally, I would like to express my sincere thanks to my family and friends for being there for me always.
## Contents

Declaration of Authorship i

Abstract ii

Acknowledgements iii

List of Figures vi

List of Tables vii

1 Introduction 1
   1.1 Background and Motivation .................................................. 1
   1.2 Organization of the Thesis .................................................. 3

2 Governing Equations 4
   2.1 Hyperbolic Conservation Laws .............................................. 4
       2.1.1 Linear Advection Equation ........................................... 6
       2.1.2 The Euler Equations .................................................. 7

3 Mathematical Formulation of the Numerical Scheme 8
   3.1 The Spectral Difference Scheme from the Discontinuous Galerkin Formu-
       lation ............................................................................. 8
   3.2 The Spectral Difference Scheme from the Strong Form of the Equation 11
   3.3 The Spectral Difference Scheme Using Raviart-Thomas Elements ...... 13
   3.4 Time Integration .................................................................. 15
       3.4.1 TVD Runge-Kutta Time Discretization ............................... 15
       3.4.2 Strong Stability Preserving Time Discretization ................. 16
       3.4.3 Implicit Time Discretization ............................................ 16

4 Stability Analysis of the New Spectral Difference Scheme 18
   4.1 Stability Analysis ................................................................. 18
   4.2 Linear Stability Analysis ...................................................... 19
       4.2.1 Linear Stability Analysis for the Spatial Discretization .......... 21
       4.2.2 Linear Stability Analysis for the Full Discretization .......... 23

5 Numerical Experiments 27
   5.1 2D Linear Advection Problem ................................................. 27
5.2 2D Euler Equations .............................................. 29
  5.2.1 Test Case 1: Subsonic Non-Lifting Flow ................. 29
  5.2.2 Test Case 2: Subsonic Lifting Flow ...................... 32

6 Conclusions and Outlook ........................................ 34

A Grid Transformation ............................................. 35
  A.1 Divergence in the Reference Domain ....................... 35

B Implementation Details of the New Spectral Difference Scheme 37
  B.1 Finding The Transfer Matrix ............................... 37
  B.2 Finding The Differentiation Matrix ....................... 38
  B.3 Treating Linear and Non-Linear Elements ................. 39
List of Figures

4.1 Influence of the scaling parameter $\alpha$ on the spectrum of the Fourier symbol $Z$ for the $RT_2$-based Spectral Difference scheme ........................................ 22
4.2 Influence of the scaling parameter $\alpha$ on the spectrum of the Fourier symbol $Z$ for the $RT_2$-based Spectral Difference scheme ........................................ 22
4.3 Influence of the scaling parameter $\alpha$ and the advection angle $\theta$ (in degrees) on the spectral radius of the Fourier symbol $Z$ for the $RT_2$-based Spectral Difference scheme ........................................ 23
4.4 $RT_1$ (top left), $RT_2$ (top right) and $RT_3$ (bottom) Elements .................... 24
4.5 Spectrum of the Fourier symbol ($Z$) for the optimal and stable choice of flux nodes for $RT_1$ (top left), $RT_2$ (top right) and $RT_3$ (bottom) elements for the advection angle $\theta = 45$ degree ........................................ 25
4.6 Influence of CFL number on different advection angles for Shu-RK3 and the 4th order SSP time stepping schemes ........................................ 26
4.7 Influence of CFL number per stage on different advection angles for Shu-RK3 and the 4th order SSP time stepping schemes ........................................ 26

5.1 Convergence plot: The variation of $l_\infty$ error with different mesh ($N$) and $RT$ elements in logarithmic scale ........................................ 28
5.2 Computational mesh (1440 elements) ........................................ 30
5.3 Convergence of the residual for $RT_1, RT_2$ and $RT_3$ schemes for $M_\infty = 0.3$ and $\alpha = 0^\circ$ (Residual vs. Number of Jacobian evaluations) ........................................ 30
5.4 Mach number contours generated using the $RT_3$ scheme for $M_\infty = 0.3$ and $\alpha = 0^\circ$ ........................................ 31
5.5 Mach number contours generated using $RT_1$ (top left), $RT_2$ (top right) and $RT_3$ (bottom) schemes for $M_\infty = 0.3$ and $\alpha = 0^\circ$ ........................................ 31
5.6 Mach number contours generated using the $RT_3$ scheme for $M_\infty = 0.4$ and $\alpha = 5^\circ$ ........................................ 32
5.7 Mach number contours generated using $RT_1$ (top left), $RT_2$ (top right) and $RT_3$ (bottom) schemes for $M_\infty = 0.4$ and $\alpha = 5^\circ$ ........................................ 33
5.8 Mach number contours generated using 4th order Discontinuous Galerkin (left) and $RT_3$ (right) schemes for $M_\infty = 0.4$ and $\alpha = 5^\circ$ ........................................ 33

B.1 Composition of linear and non-linear mapping ........................................ 39
List of Tables

4.1 CFL number when Shu-RK3 scheme is used for $RT_m$ ($m = 1, 2$ and $3$) elements ................................................................. 25
4.2 CFL number when 4th order SSP scheme is used for $RT_m$ ($m = 1, 2$ and $3$) elements ................................................................. 25
5.1 Order of accuracy and the $l_\infty$ error for different meshes for $RT_1$ discretization ................................................................. 28
5.2 Order of accuracy and the $l_\infty$ error for different meshes for $RT_2$ discretization ................................................................. 28
5.3 Order of accuracy and the $l_\infty$ error for different meshes for $RT_3$ discretization ................................................................. 28
Chapter 1

Introduction

1.1 Background and Motivation

The field of Computational Fluid Dynamics (CFD) has grown to such an extent that its tools are widely used in the engineering industries to simulate fluid flow in or around various geometries of interest. CFD methods to solve compressible flow problems, in particular, are of vital interest in the aerodynamic industry in addition to their experimental techniques, such as wind-tunnel tests, to simulate aerodynamic flows. To get engineering accuracy for the simulation results, low-order methods which use Finite Volume discretization have been used to solve compressible flows. These methods are in a mature state now with sound mathematical basis and efficient implementation techniques as a result of substantial amount of research work done in these areas.

However, low-order methods are not sufficient in solving fluid flow problems, where a high level of accuracy is needed, such as turbulent flows, aeroacoustic flows etc. To capture small scale features with low-order methods, a very high mesh resolution is needed, which makes the computation prohibitive even with the existing high computational resources. It is in this context that high-order methods such as Discontinuous Galerkin (DG) and Spectral Difference (SD) which use locally discontinuous polynomials to represent the solution field inside a mesh element became increasingly popular for smooth solutions. The order of accuracy can be increased arbitrarily by increasing the polynomial degree. Unlike low-order methods, high-order ones are able to capture small scale phenomena in the fluid flow accurately with a lower mesh resolution. Even for moderate level of
accuracy, high-order methods are potentially more efficient than low-order methods in terms of total degrees of freedom. But for such problems, low order methods are still used widely as they are proved to be reliable and stable. For high-order methods to be used in such cases, there should be algorithms which are stable, robust and easy to implement.

The present work aims at analyzing, implementing and validating a new variant of Spectral Difference scheme for hyperbolic conservation laws in particular, and showing its viability in industrial applications in which accurate and fast converging results are needed.

General formulation of the Spectral Difference scheme for solving hyperbolic conservation laws on unstructured meshes has been given by Liu et al. [1]. The scheme is essentially a pseudo-spectral method in which collocation- or nodal-based locally-discontinuous polynomial approximation of the strong form of the equation is used. The scheme has got much attention due to its simplicity in formulation and implementation [2],[3].

May [4] has demonstrated that the Spectral Difference scheme is, in fact, a particular case of Discontinuous Galerkin method [5],[6],[7],[8],[9], which in turn is well supported by mathematical basis. The SD scheme can be considered as a quadrature-free nodal Discontinuous Galerkin method. The DG method is a Finite Element method that does not enforce continuity of the solutions between the cells. Due to this discontinuous nature of the solution, codes written using DG schemes are easily parallelizable, which makes the computation efficient. However, with increasing order of accuracy, the complexity of DG schemes increases, such as the evaluation of surface and volume integrals. The Spectral Difference scheme seems to be particularly attractive as there are no surface or volume integrals to be computed. But, since the scheme has been recently proposed, it is not yet backed by sufficient mathematical foundation for its stability properties, error estimates, and so forth. The scheme has been found to be stable for one dimensional linear advection problem by Jameson [10] for all orders of accuracy in an energy norm of Sobolev type. Accuracy and stability are found to be independent of the position of the solution points in most cases, which makes the design simpler [11]. But linear stability analysis performed by Van den Abeele et al. [11] shows that the scheme is unstable for order of accuracy greater than two on triangular meshes.
The new variant of the Spectral Difference scheme, which was proposed by May and Schöberl [12], is formulated by incorporating a new interpolation technique into the standard Spectral Difference scheme. In this scheme, the flux function of the conservation law is approximated by projecting it into the Raviart-Thomas ($RT$) polynomial space, which is an incomplete polynomial space. For triangular meshes, the scheme proved stable under linear stability analysis for periodic problems for which the standard Spectral Difference scheme was found unstable [12]. Further, the $RT$ space demands fewer degrees of freedom for the same order of accuracy than the standard scheme, which means a reduction in computational cost. As part of this project, we implement the new Spectral Difference scheme to solve scalar advection equation and also Euler equations in an already existing 2D code which uses standard Spectral Difference scheme and also to extend the linear stability analysis.

1.2 Organization of the Thesis

Chapter 2 gives details on the governing equations which are solved numerically using the new Spectral Difference scheme. All the mathematical formulations involved in the derivation of both the traditional and the new Spectral Difference schemes are given in Chapter 3. At first, the derivation of the Spectral Difference scheme from the Discontinuous Galerkin framework is shown and then the derivation of the Spectral Difference scheme from the strong form of the governing equation. It is followed by the mathematical formulation of the new Spectral Difference scheme. Finally, different time integration methods used in the simulation are explained. Details about the linear stability analysis performed on the new Spectral Difference scheme are given in Chapter 4. Chapter 5 shows numerical results which are all obtained using the new Spectral Difference scheme. A summary of the thesis and an outlook are given in Chapter 6.
Chapter 2

Governing Equations

2.1 Hyperbolic Conservation Laws

In this section we consider only pure initial value problems for simplicity. The discussion of initial value problems with boundary conditions is deferred to Chapter 5. A general system of conservation laws can be written as

\[ \frac{\partial u}{\partial t} + \sum_{i=1}^{d} \frac{\partial f_i(u)}{\partial x_i} = 0, \]  
(2.1)

where \( u = (u_1, u_2, ..., u_n) \), the state variable, is a vector in \( \mathbb{R}^n \) and \( f_i \), the flux functions, define a mapping from \( \mathbb{R}^n \) into \( \mathbb{R}^n \) and \( d \) is the number of spacial dimensions. Let \( A_i = \frac{\partial f_i}{\partial u} \) be the Jacobian matrix of the \( i^{th} \) flux function. Then Eq. (2.1) can also be written in the quasi-linear form as

\[ \frac{\partial u}{\partial t} + \sum_{i=1}^{d} A_i \frac{\partial u}{\partial x_i} = 0. \]  
(2.2)

Eq. (2.1) is said to be hyperbolic, if any linear combination of the Jacobian matrices \( A_i \)'s is diagonizable with \( n \) real eigenvalues and is strictly hyperbolic if the eigenvalues are distinct. We say the function \( u \) is a classical solution to Eq. (2.1), if \( u \) is a \( C^1 \) function that satisfies the Eq. (2.1) pointwise. But we cannot guarantee a unique classical solution for non-linear hyperbolic conservation laws even if the initial solution is smooth. The inability of the partial differential equations (PDEs) to deal with such situations led to
the concept of weak formulation of the governing equations. The weak formulation of Eq. (2.1) is given as

\[
\int_{\mathbb{R}^d \times \mathbb{R}^+} \left( \frac{\partial \varphi}{\partial t} + \sum_{i=1}^{d} f_i \frac{\partial \varphi}{\partial x_i} \right) \, dx \, dt + \int_{\mathbb{R}^d} u(x, 0) \varphi \, dx = 0,
\]

(2.3)

where \( \varphi \) is a smooth function, with compact support, in some space \( \vartheta \). A function \( \varphi \) has compact support if it vanishes outside some bounded set. We say \( u \) is a weak solution to Eq. (2.3), if \( u \) satisfies Eq. (2.3) for any \( \varphi \in \vartheta \). It is clear from the above equation that the solution is not required to be differentiable and hence the weak formulation admits discontinuous solutions. We can thus look for weak solutions in a broader class of functions unlike the restricted set of solutions for the strong form of the equation.

For smooth solutions, it is straightforward to show, using integration by parts, that the weak formulation reduces to the strong formulation

\[
\int_{\mathbb{R}^d \times \mathbb{R}^+} \left( \frac{\partial u}{\partial t} + \sum_{i=1}^{d} \frac{\partial f_i (u)}{\partial x_i} \right) \varphi \, dx \, dt = 0,
\]

(2.4)

in which the solution \( u \) satisfies Eq. (2.1) pointwise. Given a surface of discontinuity on the \( x - t \) plane, if we define \( u_\pm = \lim_{\epsilon \to 0^+} (u(x, t) \pm \epsilon n) \), where \( n = (n_{x_1}, n_{x_2}, \ldots, n_{x_d}, n_t) \) is the normal on the surface of discontinuity, then it can be proved that \( u \) is a weak solution of Eq. (2.3) if and only if \( u \) is a classical solution in region where \( u \in C^1 \) and \( u \) satisfies the algebraic expression

\[
(u_+ - u_-) n_t + \sum_{j=1}^{d} (f \left( u_+ \right) - f \left( u_- \right)) n_{x_j} = 0 \tag{2.5}
\]

across jump discontinuities. Eq. (2.5) is known as the Rankine-Hugoniot condition [13]. Weak solutions are not unique and one should identify the physically admissible solutions among them. Such admissible solutions turn out to be the entropy solutions which take into account the fact that entropy increases across the discontinuity. This is the reason why compression shocks, where the normal velocity is decreased from supersonic to subsonic, are observed in nature whereas expansion shocks are not, even though both form weak solutions. To give a mathematical definition of the entropy solutions, we need to first define the entropy functions of the conservative laws. A convex function \( E(u) \) is called an entropy function of Eq. (2.1), if there exist functions \( F_i \), \( i = 1, \ldots, d \), called...
Chapter 2. Governing Equations

entropy fluxes, such that

\[ \nabla u E(u) A_i = \nabla u F_i(u), \quad i = 1, ..., d, \]  

(2.6)

where \( A_i = \frac{\partial f_i}{\partial u} \) is the Jacobian matrix of the \( i \)-th flux function. A weak solution to Eq. (2.3) is an entropy solution if \( u \) satisfies for all entropy functions \( E(u) \) the condition

\[ \int_{\mathbb{R}^d \times \mathbb{R}^+} \left( E(u) \frac{\partial \varphi}{\partial t} + \sum_{i=1}^{d} f_i \frac{\partial \varphi}{\partial x_i} \right) dx dt + \int_{\mathbb{R}^d} E(u(x,0)) \varphi \, dx \geq 0. \]  

(2.7)

It is possible to deduce that \( u \) is an entropy solution to Eq. (2.1), if the following conditions hold:

- \( u \) is a classical solution that satisfies Eq. (2.1) pointwise in regions where \( u \in C^1 \),

- \( u \) satisfies the Rankine-Hugoniot condition Eq. (2.5),

- \( u \) satisfies the entropy jump inequality,

\[ (E(u_+) - E(u_-)) n_t + \sum_{j=1}^{d} (f(u_+) - f(u_-)) n_x j \leq 0. \]  

(2.8)

Finding the entropy functions associated with the nonlinear system of conservation laws is in general not trivial. For the scalar conservation law, any convex function is an entropy function and it can be shown that the entropy solutions are unique [13].

2.1.1 Linear Advection Equation

One of the simplest hyperbolic conservation laws is the scalar advection equation which models the transport of a scalar conserved variable:

\[ \frac{\partial u(x, t)}{\partial t} + \nabla \cdot \vec{f}(u) = 0, \]  

(2.9)

where \( u \) is the scalar conserved variable and \( \vec{f} \) is the flux function. The flux function can be written as \( \vec{f} = \vec{c} u \), where \( \vec{c} = (c_1, c_2, ..., c_d) \) is known as the advection velocity.

Given initial conditions at \( t = 0 \), the analytical solution of this equation is given as

\[ u(x, t) = u(x - \vec{c} t, 0). \]  

(2.10)
From the above equation, it is clear that the solution is constant on \( \xi = x - ct \), which are called characteristics. The equation is hyperbolic as it has \( c_i \) as real eigenvalue of each flux Jacobian \( \frac{\partial f_i}{\partial u} \).

### 2.1.2 The Euler Equations

Inviscid compressible flows are modeled by Euler equations which are given in 2D in the conservative form as

\[
\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = 0, \tag{2.11}
\]

where \( \mathbf{u} \) is the state vector of conservative variables and \( f \) and \( g \) are vectors of flux functions given by

\[
\mathbf{u} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{bmatrix}, \quad f = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ u(E + p) \end{bmatrix}, \quad g = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(E + p) \end{bmatrix}, \tag{2.12}
\]

where \( \rho \) is the density of the fluid, \( u \) is the \( x \) velocity, \( v \) is the \( y \) velocity, \( p \) is the pressure, and \( E \) is the total energy. This set of four coupled and non-linear equations model the conservation of mass, \( x \) momentum, \( y \) momentum, and total energy, respectively.

To close the system of equations, we assume the fluid considered in the simulation as an ideal gas for which the relation between pressure and energy is

\[
p = (\gamma - 1) \left( E - \frac{1}{2} \rho (u^2 + v^2) \right), \tag{2.13}
\]

where \( \gamma \) is the specific heat capacity ratio and is 1.4 for air. It is possible to show under ideal gas law assumption that the flux Jacobians, \( \frac{\partial f}{\partial \mathbf{u}} \) and \( \frac{\partial g}{\partial \mathbf{u}} \), have real eigenvalues, which means Eq. (2.11) together with Eq. (2.12) form a hyperbolic system of partial differential equations.
Chapter 3

Mathematical Formulation of the Numerical Scheme

3.1 The Spectral Difference Scheme from the Discontinuous Galerkin Formulation

The Spectral Difference scheme can be derived from the weak formulation of the governing equations [4]. Here we show the derivation for the 1-dimensional case. Consider the scalar conservation equation in 1D

\[ \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \]  

(3.1)

on some domain \((x, t) \in \Omega \times \mathbb{R}^+\), where \(\Omega \subset \mathbb{R}\). Now the domain, \(\Omega\), is decomposed into \(N_T\) cells and these cells are denoted by \(\Omega_i, i = 1, ..., N_T\). For each cell \(\Omega_i\), \(x_i\) is the midpoint of the cell, \(x_{i-\frac{1}{2}}\) and \(x_{i+\frac{1}{2}}\) represent the coordinate of the left and right boundary of the cell, respectively. The volume, \(\Delta x_i\), is assumed to be same for all cells and is equal to \(\Delta x\). The weak form of Eq. (3.1), considering integration only in \(\Omega\), is given as

\[ \int_{\Omega_i} \frac{\partial u}{\partial t} \varphi (x) \, dx - \int_{\Omega_i} f(u) \varphi' (x) \, dx + [\varphi (x) f(u(x,t))]_{x=x_{i-\frac{1}{2}}}^{x=x_{i+\frac{1}{2}}} = 0, \]  

(3.2)
where \( \varphi \) is a smooth test function. The DG approximation is then to find an approximate solution \( u_h \) to the above equation such that

\[
\int_{\Omega_i} \frac{\partial u_h}{\partial t} \varphi(x) dx - \int_{\Omega_i} f(u_h) \varphi'(x) dx + h_{i+\frac{1}{2}} \varphi(x_{i+\frac{1}{2}}) - h_{i-\frac{1}{2}} \varphi(x_{i-\frac{1}{2}}) = 0, \quad \forall \varphi \in P_m, \tag{3.3}
\]

where \( h_{i-\frac{1}{2}} \) and \( h_{i+\frac{1}{2}} \) are the numerical fluxes, that approximate the analytical flux \( f(u) \), evaluated at \( x_{i-\frac{1}{2}} \) and \( x_{i+\frac{1}{2}} \), respectively, and \( P_m \) is the space of polynomials of maximum degree \( m \). We consider a linear transformation from the reference domain \((\xi)\) to the physical domain \((x)\) for each cell, which is defined by the invertible mapping \( \Phi : \xi \mapsto x \) with a non-singular Jacobian, \( J = \partial x / \partial \xi \) and the DG discretization is formulated in this reference domain. The linear mapping for each cell \( i \) is defined as \( \xi = 2(x - x_i) / \Delta x \) for \( \xi \in [-1, 1] \). We define two sets of points in the reference domain. The first set, \( \hat{\xi}_j, j = 1, \ldots, m + 1 \), is for the solution collocation and the second one, \( \tilde{\xi}_k, k = 1, \ldots, m + 2 \), is for the flux collocation. To formulate the DG discretization, the solution \( u \) in each cell is approximated to \( u_h \) by projecting it onto a finite dimensional polynomial space of degree \( m \) as

\[
u_h(\xi) = \sum_{j=1}^{m+1} u_j l_j(\xi), \tag{3.4}\]

where \( l_j(\xi), j = 1, \ldots, m + 1 \) are the Lagrangian interpolation functions with property \( l_j(\hat{\xi}_j) = \delta_{jk} \). The degrees of freedom are thus given as \( u_j = u_h(\hat{\xi}_j) \). Substituting Eq. (3.4) into Eq. (3.3) and choosing the test functions as Lagrangian functions \( l_q \) give the equation:

\[
|J| \sum_{j=1}^{m+1} \frac{du_j}{dt} \int_{-1}^{1} l_j l_q d\xi - \int_{-1}^{1} f(u)l'_q d\xi + h_{i+\frac{1}{2}} l_q(1) - h_{i-\frac{1}{2}} l_q(-1) = 0, \quad q = 1, \ldots, m + 1, \tag{3.5}\]

where \( |J| \) is the determinant of the Jacobian \( J \). The quadrature free DG method introduced by Atkins and Shu [14] is considered now for the flux approximation. The flux function \( f \) is approximated to \( f_h \) by projecting it onto a finite dimensional polynomial space of degree \( m + 1 \) using the Lagrangian interpolation functions \( \hat{l}_k \) which are defined by the flux collocation nodes \( \tilde{\xi}_k \):

\[
f_h(\xi) = \sum_{k=1}^{m+2} f_k \hat{l}_k(\xi). \tag{3.6}\]
This is precisely the nodal DG formulation considered in [15]. The difference between standard nodal DG and the Spectral Difference scheme lies in the choice of degrees of freedom for the flux interpolation. The degrees of freedom for the flux functions are chosen as follows:

\[
 f_k = \begin{cases} 
 h_{i-\frac{1}{2}}, & k = 1, \\
 f_h(u_h(\xi_k)), & k \in \{2, ..., m+1\}, \\
 h_{i+\frac{1}{2}}, & k = m+2.
\end{cases}
\]  

(3.7)

Substituting Eqns. (3.6) and (3.7) into Eq. (3.5) leads to

\[
 |J| \sum_{j=1}^{m+1} \frac{du_j}{dt} \int_{-1}^{1} l_j l_q d\xi + \sum_{k=1}^{m+2} f_k \int_{-1}^{1} \hat{l}_k \hat{\xi}_q d\xi = 0. \quad q = 1, ..., m+1.
\]  

(3.8)

If we define \( m_{q,j} = \int_{-1}^{1} l_j l_q d\xi \) and \( s_{q,k} = \frac{1}{|J|} \int_{-1}^{1} \hat{l}_k \hat{\xi}_q d\xi \) as elements in the matrices \( M \) and \( S \), respectively, then Eq. (3.8) can be rewritten as

\[
 M \frac{dU}{dt} + SF = 0,
\]  

(3.9)

where \( U = (u_1, ..., u_{m+1})^T \) is the vector with all the solution degrees of freedom and \( F = (f_1, ..., f_{m+2})^T \) is the vector with all the flux degrees of freedom. Since \( M \) is positive definite, it has an inverse and hence Eq. (3.9) can be rewritten as

\[
 \frac{dU}{dt} + M^{-1}SF = 0.
\]  

(3.10)

If we define a matrix \( D \) whose entries are given as \( d_{j,k} = \frac{1}{|J|} \hat{l}_k(\xi_j) \), then the product of matrices \( M \) and \( D \) is given as

\[
 [MD]_{q,k} = \sum_{j=1}^{m+1} m_{q,j} d_{j,k} = \frac{1}{|J|} \int_{-1}^{1} l_j \sum_{j=1}^{m+1} l_j \hat{l}_k(\xi_j) d\xi = \frac{1}{|J|} \int_{-1}^{1} l_q \hat{l}_k d\xi = s_{q,k} = [S]_{q,k}.
\]  

(3.11)

This means \( D = M^{-1}S \) and hence Eq. (3.10) can be rewritten in the final form in 1D for each cell \( i \) as

\[
 \frac{du_j}{dt} + \frac{1}{|J|} \sum_{k=1}^{m+2} \hat{l}_k(\xi_j) \hat{l}_k^{(i)} f_k = 0, \quad j = 1, ..., m+1.
\]  

(3.12)

Though the original derivation of the Spectral Difference scheme is from the strong form of the equation, it is expected that establishing the Spectral Difference scheme as a
particular kind of DG may be useful for further mathematical analysis of the scheme. Also, many established theories in the paradigm of nodal DG schemes may be applicable to the SD scheme as well.

3.2 The Spectral Difference Scheme from the Strong Form of the Equation

Here, we consider the 2-dimensional case. Similar to the 1-dimensional case, it is possible to derive the SD scheme from the weak formulation. We now present the derivation of the SD scheme from the strong form of the equation as given in the original formulation of the Spectral Difference [1]. Consider the scalar hyperbolic conservation equation

\[
\frac{\partial u(x, t)}{\partial t} + \nabla \cdot \vec{f}(u) = 0 \quad (3.13)
\]

on some domain \((x, t) \in \Omega \times \mathbb{R}^+\), where \(\Omega \subset \mathbb{R}^2\) in the present case. Consider a triangulation of the domain, \(T_h = \{T^{(i)}, i = 1, ..., N_T\}\) which decomposes the domain into \(N_T\) cells, where each cell is denoted by the index \(i\) as a bracketed superscript. However, the formulations given below hold for each cell and the superscript is omitted to avoid confusion and is shown only in the final form of the equation. We consider the transformation from the reference domain \((\xi)\) to the physical domain \((x)\) for each triangular cell which is defined by the invertible mapping \(\Phi : \xi \mapsto x\) with a non-singular Jacobian, \(J = \partial x / \partial \xi\), such that each element in the triangulation can be mapped to a reference domain \(\tilde{T} = \Phi^{-1}(T)\). Two sets of points are defined in the reference domain. The first set, \(\tilde{\xi}_j\), \(j = 1, ..., N_m\), is for the solution collocation and the second one, \(\tilde{\xi}_k\), \(k = 1, ..., N_{m+1}\), is for the flux collocation. In the reference domain, the above hyperbolic equation is of the form

\[
\frac{\partial u(x, t)}{\partial t} + \frac{1}{|J|} \nabla \cdot \left( |J| J^{-1} \vec{f}(u) \right) = 0. \quad (3.14)
\]

Derivation of the flux function in the reference domain is given in Appendix A.1.
Chapter 3. Mathematical Formulation of the Numerical Scheme

Now the solution function $u$ in the reference domain is approximated to $u_h$ by projecting it onto a finite dimensional polynomial space as

$$u_h (\xi) = \sum_{j=1}^{N_m} u_j l_j (\xi),$$

where $l_j (\xi), j = 1, \ldots, N_m$ are the Lagrangian interpolation functions, defined by the solution collocation nodes with the property $l_k (\xi_j) = \delta_{jk}$ and hence the coefficients are given as $u_j = u_h (\xi_j)$. These Lagrangian functions form a basis in the finite dimensional polynomial space of degree $m$, denoted as $P_m$. In 2D, the number of degrees of freedom required to represent a function in the space $P_m$ is given as

$$N_m = \frac{(m + 1) (m + 2)}{2}.$$  \hspace{1cm} (3.16)

The flux function in the reference domain, which is defined as $|J| J^{-1} \vec{f}$, is approximated by $\vec{f}_h$, by projecting it component-wise into a finite dimensional polynomial space of degree $m + 1$ as

$$\vec{f}_h (\xi) = \sum_{k=1}^{N_{m+1}} \vec{f}_k \hat{l}_k (\xi),$$

where $\hat{l}_k (\xi), k = 1, \ldots, N_{m+1}$ are the Lagrangian interpolation functions, defined by the flux collocation nodes with the property $\hat{l}_k (\xi_j) = \delta_{jk}$. The coefficients of the interpolation are defined as

$$\vec{f}_k = \begin{cases} 
|J| J^{-1} \vec{f} (\xi_k), & \xi_k \in \hat{T}, \\
\vec{f}_\text{num} & \hat{\xi}_k \in \partial \hat{T}, 
\end{cases}$$

where

$$\vec{f}_\text{num} \cdot n = h$$

with $n$ as the outward normal on $\partial \hat{T}$ and $h$ as a standard numerical flux function like the Roe flux or the Lax-Friedrichs flux. Note that the flux function is approximated to one degree higher than the solution function. This is to ensure that the divergence of the flux will be a polynomial of degree $m$.

Divergence of the flux function in the finite dimensional polynomial space is given as

$$\left( \nabla^\xi \cdot \vec{f}_h \right) (\xi) = \sum_{k=1}^{N_{m+1}} \left( \nabla^\xi \hat{l}_k \right) (\xi) \cdot \vec{f}_k.$$  \hspace{1cm} (3.20)
The Spectral Difference scheme can now be written for each degree of freedom of the solution function in each cell $i$ as

$$\frac{du_j^{(i)}}{dt} + \frac{1}{|J_i^{(i)}|} \sum_{k=1}^{N_{m+1}} \left( \nabla \xi_k \right) \left( \xi_j \right) \cdot \vec{f}_k^{(i)} = 0, \quad j = 1, \ldots, N_m, \quad i = 1, \ldots, N_T. \quad (3.21)$$

As mentioned in Section 1.1, the above Spectral Difference scheme was found unconditionally linearly unstable for triangles [11].

### 3.3 The Spectral Difference Scheme Using Raviart-Thomas Elements

The same hyperbolic Eq. (3.14) is considered in the reference domain. The solution function is approximated as in Eq. (3.15), which is the same as in the standard Spectral Difference scheme. For the flux interpolation, vector valued interpolation is used where the interpolation functions are vectors in the Raviart-Thomas ($RT$) space. For a degree $m$, the $RT$ space is defined as

$$RT_m = (P_m)^2 + (x,y)^T P_m. \quad (3.22)$$

For $m = 1$, the monomials $\vec{\phi}_n, n = 1, \ldots, 8$ which form a basis in the $RT$ space are given as $\{(1,0)^T, (x,0)^T, (y,0)^T, (0,1)^T, (0,x)^T, (0,y)^T, (x^2,yx)^T, (xy,y^2)^T\}$. Since $RT_m$ is the smallest space having divergence in $P_m$ [16], it reduces the number of degrees of freedom needed for flux interpolation and hence the computational cost is lesser compared to that for the traditional Spectral Difference scheme. In 2D, the number of degrees of freedom to represent a vector-valued function in the $RT$ space is given by

$$N_{m}^{RT} = (m + 1) (m + 3). \quad (3.23)$$

The flux function in the reference domain, which is defined as $|J|J^{-1}\vec{f}$, is approximated to $\vec{f}_h$ in the $RT$ space as

$$\vec{f}_h (\xi) = \sum_{k=1}^{N_{m}^{RT}} f_k \vec{\psi}_k (\xi), \quad (3.24)$$

where $\vec{\psi}_k, k = 1, \ldots N_{m}^{RT}$ are interpolating functions which form a basis in the Raviart-Thomas space. Note that the basis functions are vectors and the coefficients are scalars.
unlike the standard Spectral Difference where the basis is scalar and the coefficients are vectors. Further, these interpolation functions have the property
\[ \vec{\psi}_j (\hat{\xi}_k) \cdot s_k = \delta_{jk}, \]
where \( \hat{\xi}_k, k = 1, \ldots, N_{RT} \) are the flux collocation points and \( s_k \) are the unit vectors defined at those points. The degrees of freedom for the flux interpolation are given as
\[ f_k = \begin{cases} |J| J^{-1} \tilde{f}(\hat{\xi}_k) \cdot s_k, & \hat{\xi}_k \in \hat{T} \smallskip \hfill (3.25) \\ h, & \hat{\xi}_k \in \partial \hat{T}, \end{cases} \]
where \( h \) is a standard numerical flux. Note that the numerical flux is directly used as the degree of freedom on the boundary unlike the standard Spectral Difference where the numerical flux is used to replace the normal component of the analytical flux and is then projected into orthogonal directions to obtain the degrees of freedom [1]. To calculate the flux values, \( \tilde{f} \), at the flux collocation points, \( \hat{\xi}_k \), we have to find the solution values at those points. This is done by using a transfer matrix which is explained in Appendix B.1. The divergence of the flux function at the solution nodes is given as
\[ \left( \nabla \cdot \vec{f}_h \right)(\hat{\xi}_j) = \sum_{k=1}^{N_{RT}} f_k \left( \nabla \cdot \vec{\psi}_k \right)(\hat{\xi}_j), \quad j = 1, \ldots, N_m. \quad (3.26) \]
The values of \( \left( \nabla \cdot \vec{\psi}_k \right)(\hat{\xi}_j) \) can be written in the form of a matrix called differentiation matrix. The evaluation of the differentiation matrix is given in Appendix B.2. The new Spectral Difference scheme can now be written for each degree of freedom of the solution function in each cell \( i \) as
\[ \frac{du_{(i)}^j}{dt} + \frac{1}{|J(i)|} \sum_{k=1}^{N_m} f_k^{(i)} \left( \nabla \cdot \vec{\psi}_k \right)(\hat{\xi}_j) = 0, \quad j = 1, \ldots, N_m, \quad i = 1, \ldots, N_T. \quad (3.27) \]
The above equation is rewritten in terms of the residual, \( R \), as
\[ \frac{dU}{dt} = R(U), \quad (3.28) \]
where \( U = (u_1^{(1)}, u_2^{(1)}, \ldots, u_{N_{RT}}^{(N_m)})^T \) comprises all solution degrees of freedom in all the cells. For triangular mesh elements, this modified Spectral Difference scheme with flux interpolation using Raviart-Thomas elements was proved stable under linear stability analysis for which the standard Spectral Difference scheme was found unstable [12].
3.4 Time Integration

3.4.1 TVD Runge-Kutta Time Discretization

For time-dependent problems, higher order explicit multistage Runge-Kutta schemes by Gottlieb and Shu \cite{17} which preserve the TVD property of the spatial operator are used to integrate the system of ODEs (3.28) (TVD stability will be briefly discussed in section 4.1 in Chapter 3). TVD Runge-Kutta schemes are used for time discretization as it can be shown that a non-TVD Runge-Kutta time discretization can generate oscillations even for TVD spatial discretizations \cite{17}. We use the Runge-Kutta schemes, where the solution at \((n+1)\)-th iteration, \(U^{n+1}\), is obtained from \(U^n\) as follows.

\[
w^{(0)} = U^n,
\]

\[
w^{(k)} = \sum_{l=0}^{k-1} \alpha_{kl}w^{(l)} + \Delta t \beta_{kl}R^{(l)} \quad k = 1, ..., p,
\]

\[U^{n+1} = w^{(p)},
\]

where \(p\) is the number of intermediate stages, \(\Delta t\) is the time step and \(R^{(l)}\) is the residual evaluated at \(w^{(l)}\). Note that the bracketed superscript here stands for different stages and not for different cells. For a 3 stage \((p = 3)\) 3rd order TVD Runge-Kutta scheme (Shu-RK3), the coefficients are given in matrix form as

\[
\alpha = \begin{bmatrix}
1 \\
\frac{3}{4} & \frac{1}{4} \\
\frac{1}{3} & 0 & \frac{2}{3}
\end{bmatrix}, \quad \beta = \begin{bmatrix}
1 \\
0 & \frac{1}{4} \\
0 & 0 & \frac{2}{3}
\end{bmatrix}.
\]

Here \((l,k)\) represents the index to the matrix elements with \(l = 0, ..., k-1\) and \(k = 1, ..., p\).

And for a 2 stage, 2nd order scheme (Shu-RK2), the coefficients are given as

\[
\alpha = \begin{bmatrix}
1 \\
\frac{1}{2} & \frac{1}{2}
\end{bmatrix}, \quad \beta = \begin{bmatrix}
1 \\
0 & \frac{1}{2}
\end{bmatrix}.
\]
3.4.2 Strong Stability Preserving Time Discretization

Following the successful application of TVD Runge-Kutta schemes for hyperbolic partial differential equations, a new general class of Strong Stability Preserving (SSP) schemes was developed by Gottlieb and Shu [18]. SSP schemes, in general, maintain stability in the same norm as that of the first-order forward Euler discretization, but with a smaller time step restriction. The TVD Runge-Kutta scheme is one type of SSP scheme, where the stability is preserved with respect to the Total Variation norm. More efficient SSP schemes have been developed by Spiteri and Ruuth [19], in which the number of stages is higher than the order of accuracy and higher time steps are allowed. Such a 5 stage 4th order SSP scheme is also used in our linear stability analysis of the RT schemes. The coefficients are given in the matrix form as

\[
\alpha = \begin{bmatrix}
1 \\
0.444370494067 & 0.555629505933 \\
0.620101851385 & 0 & 0.379898148615 \\
0.178079954108 & 0 & 0 & 0.821920045892 \\
0.006833258840 & 0 & 0.517231672090 & 0.127598311333 & 0.348336757737
\end{bmatrix},
\]

(3.32)

\[
\beta = \begin{bmatrix}
0.391752227004 \\
0 & 0.368410592630 \\
0 & 0 & 0.251891774247 \\
0 & 0 & 0 & 0.544974750212 \\
0 & 0 & 0 & 0 & 0.084604163382 & 0.226007483194
\end{bmatrix}.
\]

(3.33)

3.4.3 Implicit Time Discretization

The time discretization can be written in a backward Euler form as

\[
\frac{U^{n+1} - U^n}{\Delta t} = R(U^{n+1}),
\]

(3.34)

where the residual $R$ is defined in Eqns. (3.27), (3.28). The residual is now expanded in Taylor series as follows

\[
R(U^{n+1}) = R(U^n) + \frac{dR(U^n)}{dt} \Delta t + \ldots
\]

(3.35)
We can also write the derivative term in the above equation as

\[
\frac{dR(U^n)}{dt} \Delta t = \frac{dR(U^n)}{dU} \frac{dU}{dt} \Delta t \simeq \frac{dR(U^n)}{dU} (U^{n+1} - U^n).
\] (3.36)

If we denote \((U^{n+1} - U^n)\) as \(\Delta U^n\), the implicit scheme now reduces to

\[
\left( I - \Delta t \frac{dR(U^n)}{dU} \right) \Delta U^n = \Delta t R(U^n),
\] (3.37)

where \(\frac{dR(U)}{dU}\) is the Jacobian matrix of the residual vector. The above linear system of equations at each time step has to be solved to get \(\Delta U^n\) and hence the solution \(U^{n+1}\). Note that as \(\Delta t \to \infty\), we obtain Newton iterations. The iterations of the above form with finite value for \(\Delta t\) can be interpreted as damped Newton iterations.
Chapter 4

Stability Analysis of the New Spectral Difference Scheme

4.1 Stability Analysis

For a consistent difference approximation of a well posed linear initial value problem, the numerical stability is a necessary and sufficient condition for the convergence of the solution.

- Lax Equivalence Theorem

The above well-known theorem highlights the importance of stability analysis of a numerical scheme. Numerical schemes developed for hyperbolic conservation laws in general should possess nonlinear stability properties in order to show their viability to deal with discontinuities such as shock waves in the flow. A popular way to establish nonlinear stability in 1D is to ensure that the scheme is Total Variation Diminishing (TVD) stable [20]. If $\bar{u}^n$ is the cell volume average of the solution at the $n$-th iteration, then the discrete Total Variation is defined as

$$TV (\bar{u}^n) = \sum_{i=1}^{N_T} |\bar{u}^n_{i+1} - \bar{u}^n_i|,$$

(4.1)
where \( N_T \) is the total number of cells in the 1D domain. A numerical scheme is TVD (Total Variation Diminishing) in the means, if

\[
TV(\bar{u}^{n+1}) \leq TV(\bar{u}^n). \tag{4.2}
\]

High-order methods are prone to introduce oscillations near discontinuities. A TVD stable scheme is expected to capture shocks without oscillations. Further, standard arguments can be used to establish convergence from TVD property for DG and Spectral Difference scheme \([6],[21]\). Though the TVD condition, in general, reduces the order of accuracy of the scheme to one, the original order of accuracy in the smooth regions can be maintained, but with a first order accuracy near the discontinuities. A general conservative numerical scheme can be made to satisfy TVD condition by using proper limiters. But if the numerical scheme is linearly unstable, the limiter will act on smooth regions to suppress the spurious oscillations generated by linear instabilities and thereby affecting the order of accuracy in smooth regions.

### 4.2 Linear Stability Analysis

The new variant of the Spectral Difference scheme has been subject to a linear stability analysis by May \([12]\) and the same is extended here with SSP schemes for the time discretization. The linear advection Eq. (2.9) with \( \vec{f}(u) = (u|V|\cos\theta, u|V|\sin\theta) \), for the advection angle \( \theta \in [0, \pi/2] \) and \( |V| \) being the magnitude of advection velocity is considered in a rectangular domain with periodic boundary conditions. A Cartesian mesh is created and each mesh element, identified by \((i,j)\), is formed by fusing two triangular elements and the Spectral Difference scheme based on \( RT \) elements is formulated for these triangular elements. The SD formulation in semi-discrete form, using upwind fluxes on the boundary of the elements, is given as

\[
\Delta t \dot{U}^{(i,j)} = -\nu \left( AU^{(i,j)} + BU^{(i-1,j)} + CU^{(i,j-1)} \right), \tag{4.3}
\]

where \( U = (u_1, u_2, ..., u_{2Nm})^T \) comprises all solution degrees of freedom in the Cartesian mesh element \((i,j)\). The CFL number is given as \( \nu = \frac{|V|\Delta t}{h} \), where \( h \) is the Cartesian mesh edge length. \( A, B \) and \( C \) are matrices resulting from the concatenated application of the transfer matrix (B.1), used to evaluate the solution at flux collocation nodes, and
the differentiation matrix (B.2), to evaluate the divergence of flux at solution collocation nodes. The analysis considered here is based on linear stability analysis for periodic problems [22]. The solution variable is initialized with a periodic function. The variable is then decomposed into different frequency modes by Fourier transformation and the behavior of these individual modes is analyzed. It has to be noted that the stability here is measured with respect to $l_2$-norm. Parseval theorem states that the $l_2$-norm of a function is the same in both physical and Fourier space. Hence the stability which is measured for the Fourier modes is applicable in the physical variable as well. If $\hat{U} e^{i(k_x x + k_y y)}$ is one particular mode with $k_x, k_y$ being the wave numbers in $x$ and $y$ directions, respectively, then the SD discretization for this mode will take the form

$$\Delta t \frac{d\hat{U}}{dt} = \nu Z \hat{U},$$

where $Z = -(A + B e^{-i\sigma} + C e^{i\kappa})$ is the Fourier symbol of the spatial discretization. $(\sigma, \kappa) = (k_x h, k_y h)$ defines the grid frequency. The numerical stability of Eq. (4.4) depends on the eigensystem of matrix $Z$. The above linear system of equations (Eq. (4.4)) can be decoupled by diagonalizing $Z$. If $H$ denotes the matrix whose elements are the eigenvectors of $Z$ and $\lambda_j, j = 1, ..., j_{\text{max}}$ are the corresponding eigenvalues, then the similarity transformation can be written as

$$Z = H \Lambda H^{-1},$$

where $\Lambda = \text{diag}(\lambda_1, ..., \lambda_{j_{\text{max}}})$. This transformation gives a set of independent scalar equations of the form

$$\frac{dw_j}{dt} = \lambda_j w_j,$$

where $H w = \hat{U}$ and $w$ is the vector whose elements are the new scalar variables $w_j$. The solution to Eq. (4.6) takes the form:

$$w_j(t) = w_j(0) \exp(\lambda_j t).$$

For the solution, $w_j$, to be bounded, the real part of $\lambda_j$ should be non-positive.
4.2.1 Linear Stability Analysis for the Spatial Discretization

Linear stability analysis is done to find the position of flux nodes for which the scheme is linearly stable. For spatially stable discretization, all the eigenvalues of $Z$ should have negative real part. It is found that the placement of flux nodes on the edges, by means of different scaling of Legendre-Gauss quadrature points [23], does not affect the linear stability properties for $RT_1$, $RT_2$ and $RT_3$ schemes whereas the flux node placement in the interior of the triangle has considerable effects. As mentioned in section 3.3, degrees of freedom for the flux function are determined by using both flux nodes and a unit vector at those flux nodes. Here the interiors flux points are chosen such that one point with two mutually orthogonal unit vectors form two flux nodes, which means two degrees of freedom at each point. For $RT_1$, the two interior degrees of freedom are put at the centroid and this was found to be stable. In the case of $RT_2$, there are six interior degrees of freedom (three points). The position of these three points can be varied linearly by a scaling parameter $\alpha$, such that when $\alpha = 1$ the three points coincide with the corner points and when $\alpha = 0$ the three points collapse onto the centroid of the triangle. Both $\alpha = 1$ and $\alpha = 0$ are excluded since those configurations lead to singular stencils. If $\xi^v_i$, $i = 1, 2, 3$ are the 3 vertices of the reference triangle and $\xi^c$ is the centroid, then the linear variation of the interior flux points $\xi_i$ can be written in the form

$$\xi_i = \xi^c + \alpha(\xi^v_i - \xi^c), \quad i = 1, 2, 3.$$  \hspace{1cm} (4.8)

The maximum eigenvalue of $Z$ is found numerically, considering sufficiently many grid frequencies $(\sigma, \kappa)$ and advection angles $\theta$, for different values of $\alpha$. Even though Eq. (4.3) is valid for all $\theta \in [0, \frac{\pi}{2}]$, we consider only $\theta \in [0, \frac{\pi}{4}]$ due to symmetry. Fig. 4.1 shows the maximum value of the real part of the eigenvalues ($\lambda$) of $Z$ for different values of the scaling parameter. For $\alpha < 0.5$, the discretization is unstable for all advection angles as the real part of the eigenvalues is positive for all angles. This unstable region, where there is positive real part for the eigenvalues can be observed in the plot as well. Though a stable region can be inferred from the plot for $\alpha \geq 0.5$, there is a region of instability for advection angles close to zero for a range of values of the scaling parameter $\alpha$, which is not so obvious from the plot due to low resolution. This unstable region, where the eigenvalues have very low magnitude positive real part, is shown in Fig. 4.2 which has a high resolution near $\theta = 0^\circ$. From the numerical analysis it is found that, if we consider
all possible advection angles, the discretization is stable for all advection angles only for $0.5 \leq \alpha < 0.521$.

**Figure 4.1:** Influence of the scaling parameter $\alpha$ on the spectrum of the Fourier symbol $Z$ for the $RT_2$-based Spectral Difference scheme

The maximum spectral radius of $Z$ is also calculated and is plotted for different advection angles and scaling parameters (Fig. 4.3). As shown in the plot, the spectral radius increases with the scaling parameter for all advection angles. Considering the fact that the smallest spectral radius is desirable to get the maximum stable CFL number while time integration, and the above observations on the region of stability, $\alpha = 0.5$ seems
to be the optimal choice for flux node placement for $RT_2$ discretization. Interestingly, this optimal choice corresponds to using a high-order integration rule in the interior of triangles, which is exact for polynomials of total degree 2. Similar linear stability analysis [11] showed that the 3rd order traditional Spectral Difference scheme failed in having a stable flux-point distribution, unlike the 3rd order ($RT_2$) $RT$-based Spectral Difference scheme.

![Figure 4.3: Influence of the scaling parameter $\alpha$ and the advection angle $\theta$ (in degrees) on the spectral radius of the Fourier symbol $Z$ for the $RT_2$-based Spectral Difference scheme](image)

For $RT_3$, different sets of interior points obtained by varying $\alpha$ did not give any stable discretization. However, it was found that using the points of a six-point quadrature rule [12] results in eigenvalues with non-positive real parts. It is currently unknown if this is indeed an isolated stable point, or if there exists a two parameter stability region around it. Fig. 4.4 shows the flux node distribution used for $RT_1$, $RT_2$ ($\alpha=0.5$) and $RT_3$ schemes. On the edges, the nodes are placed at the Gauss-Legendre quadrature points [23].

Fig.4.5 shows the spectrum of the Fourier symbol ($Z$) for the optimal and stable choice of flux nodes for $RT_m$, $m = 1, 2, 3$ elements for the advection angle $\theta = 45$ degree.
Chapter 4. Stability Analysis

24

\[ \hat{U}_{n+1} = G\hat{U}_n \]

\[
\| G \| \leq 1, \quad \rho \leq 1,
\]

For \( l_2 \) stability, it is sufficient to have \( \rho \leq 1 \), where \( \rho \) is the spectral radius of \( G \). In other words, for a stable time and space discretization, all the eigenvalues of \( G \) must lie inside the unit circle in the complex plane.

For a stable discretization, it is sufficient to have \( \| G \| \leq 1 \), where \( \| G \| \) is any \( p \)-norm. In that case the \( \hat{U} \) vector will remain bounded over iterations, for a bounded initial vector.

\[ G = \begin{pmatrix}
    0 & 1 & 0 & 0 \\
    0 & 0 & 1 & 0 \\
    0 & 0 & 0 & 1 \\
    1 & 0 & 0 & 0 \\
\end{pmatrix} \]

Figure 4.4: RT1 (top left), RT2 (top right) and RT3 (bottom) Elements

4.2.2 Linear Stability Analysis for the Full Discretization

Different explicit multistage time discretization methods are used for the time derivative term in Eq. (4.4). The stable flux points shown in Fig. 4.4 are used here for the linear stability analysis for the full discretization. The amplification factor \( G \), such that \( \hat{U}^{n+1} = G\hat{U}^n \), depends on parameters such as the advection angle \( \theta \), the grid frequencies \( (\sigma, \kappa) \) and the CFL number \( \nu \). For a stable discretization, it is sufficient to have \( \| G \| \leq 1 \), where \( \| G \| \) is any \( p \)-norm. In that case the \( \hat{U} \) vector will remain bounded over iterations, for a bounded initial vector. For \( l_2 \) stability, it is sufficient to have \( \rho \leq 1 \), where \( \rho \) is the spectral radius of \( G \). In other words, for a stable time and space discretization, all the eigenvalues of \( G \) must lie inside the unit circle in the complex plane. We get the maximum allowable CFL numbers by requiring that \( \rho \leq 1 \). Here \( \rho \) is taken as the maximum eigenvalue found from sufficiently many grid frequencies \( (\sigma, \kappa) \). The maximum allowable CFL numbers for different time discretization methods are found numerically for different values of advection angles \( \theta \).
It was observed that, for both $RT_2$ and $RT_3$ schemes, Shu-RK2 time discretization (Eqns. (3.29) and (3.31)) is unstable for certain advection angles. Tables 4.1 and 4.2 show the maximum stable CFL number when Shu-RK3 (Eqns. (3.29) and (3.30)) and 5-stage 4th order SSP (Eqns. (3.29), (3.32) and (3.33)) schemes were used, respectively, for a few advection angles. The CFL numbers for Shu-RK3 and SSP 4th order for

<table>
<thead>
<tr>
<th>$RT_m$</th>
<th>$\theta = 0$</th>
<th>$\theta = \pi/8$</th>
<th>$\theta = \pi/4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$RT_1$</td>
<td>0.352</td>
<td>0.289</td>
<td>0.281</td>
</tr>
<tr>
<td>$RT_2$</td>
<td>0.215</td>
<td>0.182</td>
<td>0.172</td>
</tr>
<tr>
<td>$RT_3$</td>
<td>0.140</td>
<td>0.118</td>
<td>0.108</td>
</tr>
</tbody>
</table>

$RT_2$ discretization are also plotted in Fig. 4.6. The CFL numbers for the SSP 4th order scheme are roughly 1.6 times those of the Shu-RK3. Fig 4.7 shows the CFL number
normalized with the number of stages which are 3 for Shu-RK3 and 5 for SSP 4th order. From the figure, it is clear that the computational effort for both of these time discretization is same as the two curves lie close. However, SSP 4th order scheme has got one order of accuracy higher than the Shu-RK3. So the SSP 4th order scheme can be considered to have superior performance compared to Shu-RK3.
Chapter 5

Numerical Experiments

5.1 2D Linear Advection Problem

Numerical simulations using the new Spectral Difference scheme have been performed to solve the linear advection Eq. (2.9) with \( \mathbf{f}(u) = (c_x u, c_y u) \), where \( c_x \) and \( c_y \) are the advection velocities in the \( x \) and \( y \) directions, respectively. The equation is solved for a rectangular domain, \([-1,1] \times [-1,1]\), with periodic boundary conditions. The solution field has been initialized at \( t = 0 \) as \( u(x,y) = \sin(2\pi(x+y)) \). A convergence study has been conducted using different mesh sizes for the \( RT_m \)-based Spectral Difference discretization, where \( m = 1, 2 \) and \( 3 \). The flux nodes in the reference element are distributed as shown in Fig. 4.4. The advection velocities considered were \( c_x = \cos\left(\frac{\pi}{8}\right) \) and \( c_y = \sin\left(\frac{\pi}{8}\right) \). The upwind flux was used as the numerical flux at the cell interfaces. Time integration was done using Shu-RK3 scheme. The numerical results were compared with the exact analytic solution which at any time \( t \) is given as

\[
\begin{align*}
  u(x, y, t) &= u(x - c_x t, y - c_y t, 0).
\end{align*}
\]  

Fig. 5.1 shows the \( l_\infty \) error at \( t = 0.1 \) for different mesh \( (N) \) and \( RT \) elements in logarithmic scale, where \( N = \frac{2}{h} \) with \( h \) as the characteristic length of the mesh.

Tables 5.1, 5.2 and 5.3 show \( l_\infty \) errors and orders of accuracy for different meshes and \( RT \) elements. The order of accuracy achieved here for the \( RT_m \) scheme is approximately \( m + 1 \), the optimal attainable order for smooth solutions.
Figure 5.1: Convergence plot: The variation of $l_\infty$ error with different mesh ($N$) and $RT$ elements in logarithmic scale.

Table 5.1: Order of accuracy and the $l_\infty$ error for different meshes for $RT_1$ discretization

<table>
<thead>
<tr>
<th>$N$</th>
<th>$l_\infty$ error</th>
<th>Order of accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>8.64E-2</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>1.05E-2</td>
<td>1.9184</td>
</tr>
<tr>
<td>50</td>
<td>3.78E-3</td>
<td>1.9999</td>
</tr>
<tr>
<td>80</td>
<td>1.48E-3</td>
<td>1.9950</td>
</tr>
<tr>
<td>100</td>
<td>9.47E-4</td>
<td>2.0009</td>
</tr>
</tbody>
</table>

Table 5.2: Order of accuracy and the $l_\infty$ error for different meshes for $RT_2$ discretization

<table>
<thead>
<tr>
<th>$N$</th>
<th>$l_\infty$ error</th>
<th>Order of accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.00E-2</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>3.79E-4</td>
<td>2.9790</td>
</tr>
<tr>
<td>50</td>
<td>8.23E-5</td>
<td>2.9896</td>
</tr>
<tr>
<td>80</td>
<td>2.02E-5</td>
<td>2.9887</td>
</tr>
<tr>
<td>100</td>
<td>1.03E-5</td>
<td>3.0184</td>
</tr>
</tbody>
</table>

Table 5.3: Order of accuracy and the $l_\infty$ error for different meshes for $RT_3$ discretization

<table>
<thead>
<tr>
<th>$N$</th>
<th>$l_\infty$ error</th>
<th>Order of accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>5.88E-4</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>7.86E-6</td>
<td>3.9276</td>
</tr>
<tr>
<td>50</td>
<td>1.07E-6</td>
<td>3.9037</td>
</tr>
<tr>
<td>80</td>
<td>1.59E-7</td>
<td>4.0564</td>
</tr>
<tr>
<td>100</td>
<td>6.61E-8</td>
<td>3.9335</td>
</tr>
</tbody>
</table>
5.2 2D Euler Equations

The Euler Eqns. (2.11) and (2.12) have been solved numerically on an unstructured grid for the subsonic steady-state flow over the airfoil NACA0012 using the newly formulated RT-based Spectral Difference scheme. The computational mesh (1440 elements) used for the simulation is shown in Fig. 5.2. The surface of the airfoil is approximated by cubic splines. The treatment of linear and non-linear mesh elements is given in Appendix B.3. The simulations were done using 2nd order (RT₁), 3rd order (RT₂) and 4th order (RT₃) schemes. The flux nodes in the reference element are distributed as shown in Fig. 4.4. The solution field has been initialized in such a way that both non-dimensional pressure \( p \) and density \( \rho \) have value one in the entire domain. The initial values of other solution variables are found from the free stream Mach number \( M_\infty \) and the angle of attack \( \alpha \). Slip boundary condition has been used on the surface of airfoil and free stream values on the outer boundary. Jameson’s H-CUSP flux [24] was used as the numerical flux at the cell interfaces and it provides appropriate numerical dissipation for stability. Two test cases are presented below, each with a particular Mach number and angle of attack. In both cases, time stepping was done using the implicit scheme mentioned in section 3.4.3. To solve the linear system which was obtained as a result of implicit discretization, we have used the PETSc library [25]. The basic parameters to solve the linear system using an implicit scheme are the Jacobian matrix \( \frac{dR(u)}{du} \), the solution methodology and the preconditioning of the system. The assembly of the Jacobian matrix is straightforward with the transfer matrix and differentiation matrix available for residual computation. The preconditioning of the system was done using Incomplete LU (ILU) factorization [26] and the final linear system was solved using the GMRES algorithm [27].

5.2.1 Test Case 1: Subsonic Non-Lifting Flow

Here, we consider free stream Mach number \( M_\infty = 0.3 \) and angle of attack \( \alpha = 0^\circ \). Fig. 5.3 shows the decay of the residual against number of Jacobian (Eqn. (3.37)) evaluations for RT₁, RT₂ and RT₃ schemes. Fig. 5.4 shows the contours of Mach number around the airfoil generated using the RT₃ scheme. Even with a coarse mesh, the Mach contours are well captured.
Chapter 5. Numerical Experiments

Figure 5.2: Computational mesh (1440 elements)

Figure 5.3: Convergence of the residual for RT₁, RT₂ and RT₃ schemes for $M_\infty = 0.3$ and $\alpha = 0^\circ$ (Residual vs. Number of Jacobian evaluations)

Fig. 5.5 shows the Mach number contours around the leading edge of the airfoil generated using RT₁, RT₂ and RT₃ schemes. It can be observed that the Mach number contours are better captured using the RT₃ scheme as it has got the solution with the highest polynomial degree compared to that of RT₁ and RT₂ schemes.
Figure 5.4: Mach number contours generated using the RT$_3$ scheme for $M_\infty = 0.3$ and $\alpha = 0^\circ$

Figure 5.5: Mach number contours generated using RT$_1$ (top left), RT$_2$ (top right) and RT$_3$ (bottom) schemes for $M_\infty = 0.3$ and $\alpha = 0^\circ$
5.2.2 Test Case 2: Subsonic Lifting Flow

In the second test case, we consider free stream Mach number $M_\infty = 0.4$ and angle of attack $\alpha = 5^\circ$. The computational grid used was the same as in the first test case. Fig. 5.6 shows the contours of Mach number around the airfoil generated using the $RT_3$ scheme. The Mach number contours around the leading edge of the airfoil, generated using $RT_1$, $RT_2$ and $RT_3$ schemes are shown in Fig. 5.7. Like in the previous test case, the Mach number contours are smoother for $RT_3$ scheme compared to $RT_1$ and $RT_2$ schemes because of the higher polynomial degree for the interpolation. For validation purpose, Mach number contours generated using 4th order DG scheme is shown along with 4th order new Spectral Difference ($RT_3$) in Fig. 5.8, both using 1280 mesh elements. As one can observe from the figure, the Mach number contours generated using the new Spectral Difference scheme looks almost same as that generated using the DG method.

![Figure 5.6: Mach number contours generated using the $RT_3$ scheme for $M_\infty = 0.4$ and $\alpha = 5^\circ$](image-url)
Figure 5.7: Mach number contours generated using RT$_1$ (top left), RT$_2$ (top right) and RT$_3$ (bottom) schemes for $M_\infty = 0.4$ and $\alpha = 5^\circ$.

Figure 5.8: Mach number contours generated using 4th order Discontinuous Galerkin (left) and RT$_3$ (right) schemes for $M_\infty = 0.4$ and $\alpha = 5^\circ$. 
Chapter 6

Conclusions and Outlook

A new variant of the Spectral Difference method which uses Raviart-Thomas elements has been implemented and validated. An existing linear stability analysis study has been extended with an optimal 5 stage 4th order Strong Stability Preserving (SSP) time discretization scheme. The SSP scheme is found to have better performance when compared with 3rd order Shu-RK3 scheme. A convergence study has been conducted with the new Spectral Difference scheme for a linear advection problem in the 2-dimensional case. Simulations were done using the 2nd, 3rd and 4th order new Spectral Difference scheme. The results show that full order of convergence is achieved with the scheme. This motivated us to perform simulations using the new scheme for the more complex case of 2D flow over an airfoil. The Euler equations have been solved around the NACA0012 airfoil for subsonic flow cases. Promising results were obtained using the new Spectral Difference scheme, which prove the viability of the scheme to be used for more practical problems.

Future work should aim at finding a more general set of stable flux nodes for the 4th, and higher order new SD schemes. For solving real life compressible fluid flow problems, the scheme should be equipped with methodologies to deal with discontinuities, like shock waves, in the flow. Furthermore, the scheme needs to be extended to solve the compressible Navier-Stokes equations. These challenges are left for future investigations.
Appendix A

Grid Transformation

A.1 Divergence in the Reference Domain

In 2D, we consider the transformation from the reference domain to the physical domain by the mapping $\Phi : (\xi, \eta) \rightarrow (x, y)$. The differentials in the physical domain and reference domain are related as

$$
\begin{pmatrix}
\frac{dx}{d\xi} \\
\frac{dy}{d\eta}
\end{pmatrix} = J
\begin{pmatrix}
\frac{d\xi}{d\eta} \\
\frac{d\eta}{d\xi}
\end{pmatrix},
$$

(A.1)

where $J$ is the Jacobian of the transformation, which is defined as

$$
J = \begin{pmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\
\frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta}
\end{pmatrix}.
$$

(A.2)

We can also write the inverse relation as

$$
\begin{pmatrix}
\frac{d\xi}{d\eta} \\
\frac{d\eta}{d\xi}
\end{pmatrix} = \begin{pmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\
\frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y}
\end{pmatrix}
\begin{pmatrix}
\frac{dx}{d\xi} \\
\frac{dy}{d\eta}
\end{pmatrix}.
$$

(A.3)

From the above equations and considering the inverse of the Jacobian, $J^{-1}$, we get the following results.

$$
\frac{\partial \xi}{\partial x} = \frac{1}{|J|} \frac{\partial y}{\partial \eta}, \quad \frac{\partial \eta}{\partial x} = -\frac{1}{|J|} \frac{\partial x}{\partial \eta}, \quad \frac{\partial \xi}{\partial y} = -\frac{1}{|J|} \frac{\partial y}{\partial \xi}, \quad \frac{\partial \eta}{\partial y} = \frac{1}{|J|} \frac{\partial x}{\partial \xi}.
$$

(A.4)

where $|J|$ is the determinant of the Jacobian matrix. Using the above results, we derive the relation between the divergence of the flux vector in the physical domain and that
in the reference domain

\[ \nabla^x \cdot \vec{f} = \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} \]

\[ = \frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial f}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial g}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial g}{\partial \eta} \frac{\partial \eta}{\partial y} \]

\[ = \frac{1}{|J|} \left( \frac{\partial f}{\partial \eta} \frac{\partial y}{\partial \eta} - \frac{\partial f}{\partial \xi} \frac{\partial y}{\partial \xi} - \frac{\partial g}{\partial \xi} \frac{\partial x}{\partial \xi} + \frac{\partial g}{\partial \eta} \frac{\partial x}{\partial \eta} \right) \]

\[ = \frac{1}{|J|} \left( \left( \frac{\partial}{\partial \xi} \left( \frac{\partial y}{\partial \eta} \right) - \frac{\partial^2 y}{\partial \xi \partial \eta} \right) - \left( \frac{\partial}{\partial \eta} \left( \frac{\partial y}{\partial \xi} \right) - \frac{\partial^2 y}{\partial \eta \partial \xi} \right) - \left( \frac{\partial}{\partial \xi} \left( \frac{\partial x}{\partial \eta} \right) - \frac{\partial^2 x}{\partial \eta \partial \xi} \right) \right) \]

\[ + \frac{1}{|J|} \left( \frac{\partial}{\partial \eta} \left( \frac{\partial x}{\partial \eta} \right) - \frac{\partial^2 x}{\partial \eta \partial \xi} \right) \]

\[ = \frac{1}{|J|} \left( \frac{\partial}{\partial \xi} \left( \frac{\partial y}{\partial \eta} \right) - \frac{\partial}{\partial \eta} \left( \frac{\partial y}{\partial \xi} \right) - \frac{\partial}{\partial \xi} \left( \frac{\partial x}{\partial \eta} \right) + \frac{\partial}{\partial \eta} \left( \frac{\partial x}{\partial \xi} \right) \right) \]

\[ = \frac{1}{|J|} \left( \frac{\partial}{\partial \xi} \left( \frac{\partial y}{\partial \xi} \right) \mid J \mid + g \frac{\partial \xi}{\partial y} \frac{\partial^2 y}{\partial \eta \partial \xi} \right) + \frac{\partial}{\partial \eta} \left( g \frac{\partial^2 y}{\partial \eta \partial \xi} \mid J \mid + f \frac{\partial^2 y}{\partial \eta \partial x} \mid J \mid \right) \]

\[ = \frac{1}{|J|} \left( \frac{\partial}{\partial \xi} \left( \mid J \mid \left( f \frac{\partial \xi}{\partial x} + g \frac{\partial \xi}{\partial y} \right) \right) + \frac{\partial}{\partial \eta} \left( \mid J \mid \left( g \frac{\partial \xi}{\partial y} + f \frac{\partial \xi}{\partial x} \right) \right) \right) \]

\[ = \frac{1}{|J|} \nabla^\xi \cdot \left( \mid J \mid J^{-1} \vec{f} \right). \]

(A.5)
Appendix B

Implementation Details of the New Spectral Difference Scheme

B.1 Finding The Transfer Matrix

As given in section 3.2, the solution function is approximated as

$$u_h(\xi) = \sum_{j=1}^{N_m} u_j l_j(\xi).$$  \hspace{1cm} (B.1)

If $\hat{\xi}_j$ are the solution nodes, then the coefficients are given as $u_h(\hat{\xi}_j) = u_j$. If the flux nodes are denoted as $\tilde{\xi}_k$, then the solution variable at flux nodes is given as

$$u_h(\tilde{\xi}_k) = \sum_{j=1}^{N_m} u_j l_j(\tilde{\xi}_k).$$  \hspace{1cm} (B.2)

Here $l_j(\tilde{\xi}_k)$, the Lagrangian polynomials evaluated at the flux nodes, are unknowns and are found as given below using the Dubiner basis functions, $\chi(\xi)$, which is a well-known orthogonal basis for triangles [28]. The values of $l_j(\tilde{\xi}_k)$ can be written in the form of a matrix which is called the transfer matrix. The Dubiner basis is obtained from the tensor product of Jacobi polynomials which are defined in the 1D interval [-1,1]. These functions can also be expressed in terms of Lagrangian functions as

$$\chi(\xi) = \sum_{j=1}^{N_m} \chi_j l_j(\xi).$$  \hspace{1cm} (B.3)
where \( \chi_j = \chi(\hat{\xi}_j) \) is evaluated at the solution points. Note that the above equation is an exact relation as both set of functions form a basis in the same polynomial space. The Dubiner basis functions can be evaluated at the flux nodes:

\[
\chi(\hat{\xi}_k) = \sum_{j=1}^{N_m} \chi_j l_j(\hat{\xi}_k). \tag{B.4}
\]

Since the Dubiner basis functions at the flux nodes \( \chi(\hat{\xi}_k) \) and those at the solution nodes \( \chi(\hat{\xi}_j) \) are known, the transfer matrix \( l_j(\hat{\xi}_k) \) is obtained by solving the linear system (B.4) for each distinct flux node \( \hat{\xi}_k \). This transfer matrix is used to find the solution at the flux nodes. Since the mesh elements, including the curved ones on the boundary, are mapped to the reference element with the same solution and flux node distribution, the transfer matrix is universal, independent of the cell and so it needs to be stored only once, which is, for the reference element.

### B.2 Finding The Differentiation Matrix

The vector-valued interpolation basis functions, \( \vec{\psi}_k \), and their derivatives can be found by using the fact that any monomial in the Raviart-Thomas (RT) space can be expressed as a linear combination of those basis functions.

\[
\vec{\phi}_n(\hat{\xi}_j) = \sum_{k=1}^{N_{RT}} a_{n,k} \vec{\psi}_k(\hat{\xi}_j), \tag{B.5}
\]

\[
\nabla^{\xi} \cdot \vec{\phi}_n(\hat{\xi}_j) = \sum_{k=1}^{N_{RT}} a_{n,k} \left( \nabla^{\xi} \cdot \vec{\psi}_k \right)(\hat{\xi}_j), \tag{B.6}
\]

where \( a_{n,k} = \vec{\phi}_n(\hat{\xi}_k) \cdot s_k \) and \( \vec{\phi}_n, n = 1, 2, ..., N_{RT} \) are the known monomial basis in the RT space. In Eq. (B.6), since the left hand side and \( a_k \) are known, the divergence of the basis functions \( \left( \nabla^{\xi} \cdot \vec{\psi}_k \right)(\hat{\xi}_j) \) can be obtained by solving the linear system in the same way as for the transfer matrix.
B.3 Treating Linear and Non-Linear Elements

Linear mesh elements are mapped to the reference element by the linear transformation which is given below.

\[
\begin{align*}
  x &= x_1 + (x_2 - x_1)\xi + (x_3 - x_1)\eta, \\
  y &= y_1 + (y_2 - y_1)\xi + (y_3 - y_1)\eta,
\end{align*}
\]  

(B.7) (B.8)

where \((x_1,y_1),(x_2,y_2)\) and \((x_3,y_3)\) are the vertices of the triangle in the physical domain. The Jacobian of this transformation, \(J\), is given in Eq. A.2.

To treat curved boundaries, we need to have non-linear mesh elements in addition to the linear mesh elements. Non-linear elements are mapped to the reference domain by composition of two mappings as shown in Fig. B.1. The first one is the linear mapping defined by \(\Xi : (r,s) \mapsto (x,y)\) with Jacobian \(J_\Xi\) and the second one is the non-linear mapping defined by \(\Phi : (\xi,\eta) \mapsto (r,s)\) with Jacobian \(J_\Phi\). The linear mapping is given as

\[
\begin{align*}
  x &= x_1 + (x_2 - x_1)r + (x_3 - x_1)s, \\
  y &= y_1 + (y_2 - y_1)r + (y_3 - y_1)s.
\end{align*}
\]  

(B.9) (B.10)

The non-linear mapping used in the present implementation was quadratic. The combined Jacobian of the full transformation is given as \(J = J_\Xi J_\Phi\). To evaluate the residual using the new Spectral Difference scheme, we need to find the projected flux function \(|J|J^{-1}f\left(\tilde{\xi}_k\right)\cdot \tilde{s}_k\) (Eq. 3.25) which is calculated at all flux points. This expression for the projected flux function is rewritten as \(f\left(\tilde{\xi}_k\right)\cdot \tilde{s}_k\), where \(\tilde{s}_k = |J|J^{-T}s_k\). In the present
implementation, we store $\tilde{s}_k$ at all flux points for the non-linear elements.

$$\tilde{s}_k = |J|J^{-T}s_k = |J_\Xi||J_\Phi|(J_\Phi^{-1}J_\Xi^{-1})^T s_k = |J_\Xi||J_\Phi|J_\Xi^{-T}J_\Phi^{-T}s_k,$$

(B.11)

where

$$|J_\Xi|J_\Xi^{-T} = \begin{pmatrix}
  y_3 - y_1 & -(y_2 - y_1) \\
  -(x_3 - x_1) & x_2 - x_1
\end{pmatrix}$$

(B.12)

and

$$|J_\Phi|J_\Phi^{-T} = \begin{pmatrix}
  \frac{\partial s}{\partial \eta} & -\frac{\partial s}{\partial \xi} \\
  -\frac{\partial r}{\partial \eta} & \frac{\partial r}{\partial \xi}
\end{pmatrix}.$$
Bibliography


