

Continuous-Galerkin Summation-by-Parts Discretization of the Khokhlov-Zabolotskaya-Kuznetsov Equation with Application to High-Intensity-Focused Ultrasound

by

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A thesis
presented to the University of Waterloo
in fulfillment of the
thesis requirement for the degree of
Master of Mathematics
in
Applied Mathematics

Waterloo, Ontario, Canada, 2024

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Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

Over the last two decades, High Intensity Focused Ultrasound (HIFU) has emerged as a promising non-invasive medical approach for locally and precisely ablating tissue, offering versatile applications in tumor treatment, drug delivery, and addressing brain disorders such as essential tremor. Its advantages include targeted energy delivery with no effect on skin integrity, low system maintenance costs, minimal impact on normal tissues, and swift recovery. Despite its merits, HIFU remains underutilized, primarily employed in specific breast cancer and prostate cancer treatments. To expand its range of applicability, a comprehensive understanding of the interaction between the ultrasound beam and local tissues at the focal point is essential. This thesis focuses on modeling critical nonlinear effects in the thermal modulation of local tissues by numerically solving the Khokhlov-Zabolotskaya-Kuznetsov (KZK) equation—which is an excellent model for the nonlinear acoustic field arising in HIFU.

Constructing high-order stable discretizations of the KZK equations poses significant challenges due to the presence of polynomial nonlinear terms and a second derivative of an integral term within this equation. Employing a continuous Galerkin approach, an operator is formulated to approximate the integral term, facilitating the construction of a modified second derivative operator. This establishes a clear correspondence between continuous and discrete stability proofs. Additionally, a skew-symmetric splitting technique is used to discretize the nonlinear advective term. The resulting semi-discrete scheme is proven to be stable. Numerical experiments using the method of manufactured solutions demonstrate the high-order accuracy and stability of the proposed numerical method. Finally, a HIFU verification test case demonstrates the applicability of the proposed scheme to investigate HIFU.

Acknowledgements

I would like to extend my deepest gratitude to my supervisors, Professor David Del Rey Fernández and Professor Sivabal Sivaloganathan, for their exceptional guidance and unwavering support throughout my master’s research. Their profound knowledge and insightful advice were instrumental in the completion of this thesis.

I am also sincerely grateful to Andrew Winters at Linköping University for his expert guidance and constructive feedback, which significantly enhanced the quality of my work.

I wish to thank my lab colleagues, Vyom Patel and Anita Gjesteland, whose contributions were invaluable. Vyom’s expertise in code optimization was crucial to the success of this project, while Anita’s assistance with theoretical aspects laid the groundwork for much of my research.

I am fortunate to have had the support of my friends, Dongze Li and Ruikun Zhou, whose encouragement made this journey more enjoyable.

Lastly, I want to express my deepest love and appreciation to my boyfriend, Jinxin Liu, for his steadfast support and companionship, both in life and in the many hours spent assisting with coding challenges.

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List of Symbols

$\mathcal{D}, \mathcal{B}, \mathcal{I}$	Differential, boundary, and initial operators, respectively
Ω, Γ	Domain and boundary
x_L, x_R	Left and right end points of the domain in one dimension, respectively
$\mathcal{F}$	Forcing term
$\mathcal{G}, \mathcal{N}$	Boundary condition and initial condition, respectively
a	Constant from the linear advection equation
$\mathcal{U}, \mathcal{V}$	Continuous function
T	Final time
x, y, z, t	Spatial and time coordinates
$\mathbf{u}, \mathbf{v}$	Restriction of the continuous functions $\mathcal{U}$ and $\mathcal{V}$ onto a nodal distribution
$\mathbf{u}_1, \mathbf{u}_n, \mathbf{v}_1, \mathbf{u}_n$	Value at the first and last node of the vectors $\mathbf{u}, \mathbf{v}$
$\ \mathbf{u}\ _2$	L_2 norm of $\mathbf{u}$
$\mathcal{L}_i(x)$	The i^{th} Lagrange basis function
$\mathbf{x}^k$	Restriction of the monomial x^k onto the nodal distribution
ξ	Computational coordinate
n	Number of nodes per element
N	Number of elements
l	Total number of nodes
$\bar{\mathbf{D}}_x$	One dimensional local SBP operator, approximating the first derivative, where $\bar{\mathbf{D}}_x = \bar{\mathbf{P}}_x^{-1} \bar{\mathbf{Q}}_x$
$\bar{\mathbf{P}}_x$	One dimensional local norm matrix, s.t. $\mathbf{u}^T \bar{\mathbf{P}}_x \mathbf{v} \approx \int_x \mathcal{U} \mathcal{V} dx$.
$\bar{\mathbf{Q}}_x$	One dimensional local transpose of the stiffness matrix operator, s.t. $\mathbf{u}^T \bar{\mathbf{Q}}_x \mathbf{v} \approx \int_x \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} dx$.

$\bar{\mathbf{M}}_\xi$	One dimensional local operator s.t. $\bar{\mathbf{M}}_\xi \mathbf{u} \approx \int_{\xi_{min}}^\xi \mathcal{U} d\xi$.
$\bar{\mathbf{E}}_x$	One dimensional local unit-normal weighted surface integration operator, s.t. $\bar{\mathbf{E}}_x = \mathbf{t}_R^T \mathbf{t}_R - \mathbf{t}_L^T \mathbf{t}_L$, $\mathbf{u}^T \bar{\mathbf{E}}_x \mathbf{v} \approx \mathbf{v}_n \mathbf{u}_n - \mathbf{v}_1 \mathbf{u}_1$.
$\mathbf{t}_L$	One dimensional local left boundary interpolation operator, s.t. $\mathbf{t}_L^T \mathbf{u} = \mathbf{u}_1$
$\mathbf{t}_R$	One dimensional local right boundary interpolation operator, s.t. $\mathbf{t}_R^T \mathbf{u} = \mathbf{u}_n$
$\mathbf{V}$	Vandermonde matrix
$\bar{\mathbf{D}}_{xg}$	One dimensional SBP global operator, approximating the first derivative, where $\bar{\mathbf{D}}_{xg} = \bar{\mathbf{P}}_{xg}^{-1} \bar{\mathbf{Q}}_{xg}$
$\bar{\mathbf{P}}_{xg}$	One dimensional global norm operator, s.t. $\mathbf{u}^T \bar{\mathbf{P}}_{xg} \mathbf{v} \approx \int_x \mathcal{U} \mathcal{V} dx$.
$\bar{\mathbf{Q}}_{xg}$	One dimensional global transpose of the stiffness matrix operator, s.t. $\mathbf{u}^T \bar{\mathbf{Q}}_{xg} \mathbf{v} \approx \int_x \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} dx$.
$\tilde{\mathbf{M}}$	See (3.48)
$\mathbf{R}_i$	Mapping matrices for the i^{th} element
$\bar{\mathbf{M}}_{\xi g}$	One dimensional global operator s.t. $\bar{\mathbf{M}}_\xi \mathbf{u} \approx \int_{\xi_{min}}^\xi \mathcal{U} d\xi$.
$\bar{\mathbf{A}}_{xg}$	One dimensional global operator s.t. $\mathbf{v}^T \bar{\mathbf{A}}_x \mathbf{u} \approx \int_x \frac{\partial \mathcal{V}}{\partial x} \frac{\partial \mathcal{U}}{\partial x} dx$.
$\bar{\mathbf{D}}_{2xg}$	One dimensional global operator, approximating second derivative, where $\bar{\mathbf{D}}_{2xg} := \bar{\mathbf{P}}_{xg}^{-1} (-\bar{\mathbf{A}}_{xg} + \bar{\mathbf{E}}_{xg} \bar{\mathbf{D}}_{xg})$
c_0	Sound speed
β	Coefficient of nonlinearity
ρ	Ambient
μ	Shear viscosity
μ_β	Bulk viscosity
c_v	Specific heat at constant volume
c_p	Specific heat at constant pressure
ω_0	Working frequency
α_0	Thermoviscous coefficient at the working frequency
p_0	Peak pressure
$\bar{z}$	Wave shock formation distance
t	Time
z	Wave propagation of the KZK equation
t'	Retarded time ,and $t' = t - \frac{z}{c_0}$
∂_τ^{-1}	Inverse operator in the KZK equation, $\partial_\tau^{-1} f ds := \int_{\tau_{min}}^\tau f ds$
$\tilde{N}, A, G_x, G_y$	Dimensionless coefficients from KZK equation
G_{xs}, G_{ys}	Coefficients from the source term of the KZK equation

X, Y, τ	Cartesian coordinates of the dimensionless form of the KZK equation
$\mathcal{P}$	Normalized pressure, $\mathcal{P}(X, Y, \tau)$ is the solution to the dimensionless form of the KZK equation
σ	Normalized wave propagation direction of ultrasound beams
X_{min}, X_{max}	Left and right boundary of domain for the dimensionless form of the KZK equation, respectively
$\otimes$	Tensor product
$\mathbf{D}_X$	Three dimensional SBP operator approximating the first derivative, where $\mathbf{D}_X = \mathbf{P}^{-1}\mathbf{Q}_X$.
$\mathbf{P}$	Three dimensional norm operator s.t. $\mathbf{u}^T \mathbf{P} \mathbf{v} \approx \int_{\Omega} \mathcal{U} \mathcal{V} d\Omega$.
$\mathbf{Q}_X$	Three dimensional transpose of the stiffness matrix operator s.t. $\mathbf{u}^T \mathbf{Q}_X \mathbf{v} \approx \int_{\Omega} \mathcal{U} \frac{\partial \mathcal{V}}{\partial X} d\Omega$.
$\mathbf{A}_X$	Three dimensional operator s.t. $\mathbf{u}^T \mathbf{A}_X \mathbf{v} \approx \int_{\Omega} \frac{\partial \mathcal{U}}{\partial X} \frac{\partial \mathcal{V}}{\partial X} d\Omega$.
$\mathbf{E}_X$	Three dimensional unit-normal weighted surface integration operator s.t. $\mathbf{E}_X = \mathbf{Q}_X + \mathbf{Q}_X^T = \mathbf{R}_{X_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{X_{max}} - \mathbf{R}_{X_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{X_{min}}, \mathbf{u}^T \mathbf{E}_X \mathbf{v} \approx \int_{\Gamma} \mathcal{U} \mathcal{V} n_X d\Gamma$.
$\mathbf{M}_{\tau}$	Three dimensional operator s.t. $\mathbf{M}_{\tau} \mathbf{u} \approx \int_{\tau_{min}}^{\tau} \mathcal{U} d\tau$.
$\mathbf{P}_{XY}$	Two dimensional norm operator s.t. $\mathbf{u}^T \mathbf{P}_{XY} \mathbf{v} \approx \int_{X_{min}}^{X_{max}} \int_{Y_{min}}^{Y_{max}} \mathcal{U} \mathcal{V} dX dY$.
$\tilde{D}_{2X}$	Modified second derivative operator $\tilde{D}_{2X} := \mathbf{P}^{-1}(-\mathbf{M}_{\tau}^T \mathbf{D}_{\tau}^T \mathbf{A}_X + \mathbf{E}_X \mathbf{D}_X)$.
$\ \mathbf{e}\ _{\mathbf{P}}$	Approximating the L_2 norm of error $\mathbf{e}$ in three dimension.

List of Abbreviations

CG	Continuous Galerkin
DG	Discontinuous Galerkin
FD	Finite Difference
GL	Gauss-Lobatto
HIFU	High-Intensity Focused Ultrasound
KZK	Khokhlov-Zabolotskaya-Kuznetsov
LHS	Left Hand Side
PDE	Partial Differential Equation
RHS	Right Hand Side
RK	Runge Kutta
SBP	Summation-by-Parts
SAT	Simultaneous Approximation Terms

Chapter 1

Introduction

In this chapter, we provide a brief overview of high-intensity focused ultrasound (HIFU) and its application. In this thesis, we utilize the Khokhlov-Zabolotskaya-Kuznetsov (KZK) equation [4] to simulate the wave propagation characteristics of HIFU, which contains the effects of diffraction, absorption and nonlinearity. Subsequently, we explore the various numerical methodologies previously employed in the context of the KZK equation and then introduce the method and tools we use in the thesis. Finally, we provide an outline of thesis.

1.1 High-Intensity Focused Ultrasound

HIFU is a non-invasive therapeutic technique, which generates high temperature around the targeted tissue by using focused ultrasound. Over the last two decades, HIFU has emerged as a promising non-invasive medical approach for locally and precisely ablating local tissue with applicability to tumor treatment, drug delivery, and addressing brain disorders (e.g., essential tremor) [73, 87, 63]. HIFU offers several advantages over other treatment alternatives [28]. Compared to open surgery for tumor resection, extracorporeal HIFU treatments do not require surgical intervention [29]. This means HIFU avoids complications such as hemorrhaging, allows for outpatient procedures without general anesthesia, and significantly reduces recovery time [75, 31]. Additionally, most HIFU systems are equipped with control software that focuses the treatment to prevent damage to adjacent organs and tissues [31]. Compared to radiation-based treatments, HIFU is a safer alternative [30]. Despite its merits, HIFU remains underutilized, primarily employed in specific breast cancer and prostate cancer treatments [74, 20]. To expand its range of ap-

plicability, a detailed understanding of the interaction between the ultrasound beam and local tissue at the focal point is essential.

In this thesis, we develop numerical methods to gain a better understanding of HIFU. Specifically, we utilize the KZK equation to model the propagation of pressure waves emanating from HIFU transducers. The KZK equation is a fundamental mathematical model that describes the propagation of finite amplitude sound waves in thermoviscous fluids. It is particularly relevant to our study as it provides a model for nonlinear effects that occur in HIFU.

1.2 Numerical methods for KZK equation

The KZK equation was first proposed in the early 1970s by R. V. Khokhlov and O. V. Zabolotskaya, with further contributions by V. P. Kuznetsov [77]. It was developed to explain the nonlinear behavior of sound beams as they travel through a medium that exhibits both thermal and viscous properties.

Historically, finite-difference and spectral methods have been popular choices for numerically solving the KZK equation. For example, in a series of papers Bakhvalov et al. [4, 6, 7, 8, 5] developed both frequency domain spectral methods and time domain FD methods to solve the KZK equation. Later, in 1993, Lee and Hamilton [55, 56] designed an operator-splitting time-domain FD method to solve the KZK equation in cylinder coordinates for pulsed, axisymmetric, finite amplitude sound beams having arbitrary spatial distributions of amplitude and phase at the source. Then Yang et al. [95] and Hajihasani et al. [45] extended Lee and Hamilton’s framework to Cartesian coordinates.

More recently, in 2017, Chou et al. [17] proposed a local discontinuous Galerkin (DG) method to solve the KZK equation, which used piecewise polynomials in each element and enables high-order in space. In this thesis, instead, we use a continuous Galerkin (CG) approach to solve KZK equation based upon the summation-by-parts (SBP) framework discussed in the next section.

1.2.1 Summation-by-Parts Operators and Simultaneous Approximation Terms

High-order methods are known to be more efficient than low-order methods as they produce less error per degree of freedom [54, 86]. However, for nonlinear problems, high-order methods can suffer from stability issues. The summation-by-parts (SBP) framework has

emerged as straightforward approach to developing provably-stable schemes for linear and variable coefficient problems (see the two review papers [35, 85]). The essential feature of SBP methods is that they mimic integration by parts, which is a key step in many stability proofs.

The foundational theory of first derivative SBP operators was established by Kreiss and Scherer [53] in 1974. They aimed to show stability for higher-order FD discretizations through the energy method. They constructed SBP operators by using centered difference stencils of order $2p$ at interior mesh nodes and special non-centered stencils near and at the mesh boundary. This theory was then extended by Strand [79] who provided existence and accuracy theorems for FD-SBP operators. More recently, Gassner [40] extended the SBP notion to collocated tensor-product DG methods on Gauss–Lobatto (GL) nodes, while Del Rey Fernández et al. [24] developed a general theory of one-dimensional SBP operators on nearly arbitrary nodal distributions. In the last number of years, these notions have been extended to encompass very general operators on unstructured meshes, for both discontinuous and continuous approaches, affording much of the flexibility associated with finite-element methods as well as the development of provably-stable schemes for nonlinear conservation laws (e.g., see [21, 14, 46]).

While SBP operators mimic integration by parts, they have no mechanism to impose boundary conditions or couple elements within a mesh. Fortunately, Funaro and Gottlieb [38, 39] introduced a penalty approach to weakly impose boundary conditions, meaning the PDE and its boundary conditions are combined at the boundary nodes. These ideas were later refined by Carpenter et al. [11] resulting in the simultaneous approximation terms (SATs) approach. The SAT method was subsequently extended and applied to various boundary and interface conditions in curvilinear coordinates [12, 69, 70] and is the predominant approach in the SBP community.

1.3 Outline of Thesis

In this thesis, we develop a continuous Galerkin (CG)-SBP-SAT provably-stable discretization of the KZK equation, which is a nonlinear wave equation that can be used to model the absorption and diffraction effect of waves from HIFU.

In Chapter 2, we will review the notion of well-posedness. In this thesis, we use the SBP-SAT approach to construct provably-stable discretizations whose stability is proven in a one-to-one fashion relative to the continuous stability analysis. In this chapter, we illustrate the type of continuous stability analysis that is employed through three equations,

namely the linear advection equation, the linear diffusion equation, and Burgers' equation, which have terms in common with the KZK equation.

In Chapter 3, the definition of SBP operators is introduced. These operators mimic integration by parts, which is a key step in the stability analysis of all of the PDEs considered in this thesis. We show how to construct local SBP operators and then explain how to extend the local operators to global one-dimensional operators using a CG approach. Moreover, we demonstrate how to use SBP operators to discretize the linear advection equation, linear diffusion equation, and the Burgers' equation with SATs to weakly impose boundary conditions. The resultant semi-discrete forms are shown to be stable, and provide motivation for the discretization of the KZK equations proposed in this thesis.

In the Chapter 4, which represents the main contribution of this thesis, we introduce the KZK equation and stability analysis. Specifically, the focus is on the dimensionless form of KZK equation. Next, we extend the one-dimensional global CG operators to three dimensions using tensor products and prove that the resultant operators are SBP. These operators are used to discretize the various terms of the KZK equations in a similar manner to that used for the linear advection equation, the linear diffusion equation, and Burgers' equation. Of particular importance, we introduce a modified second-derivative term and demonstrate that it is SBP (this is a key contribution of this thesis). Appropriate SAT terms are constructed to impose Neumann and Dirichlet boundary conditions and the resulting semi-discrete form is proven to be stable.

In Chapter 5, the convergence, accuracy, and stability properties of the proposed discretization are characterized using the method of manufactured solution. Finally, a HIFU test case inspired from [55] is numerically solved using the proposed discretization, demonstrating its applicability to investigating HIFU. Finally, conclusions and future work are discussed in Chapter 6.

Chapter 2

Well Posedness and Stability

In this chapter, we introduce the definition of well posed problems and illustrate how to prove stability by examining three PDEs, namely the linear advection equation, the linear advection-diffusion equation, and the inviscid Burgers' equation. The analysis used for these three equations are representative of the type of stability analysis that will be performed in the chapter on the KZK equations.

2.1 Well Posedness

In 1902, Jacques Hadamard [44] introduce the notion of a well posed problem and the three criteria to determine if a problem is well posed as follows:

Definition 2.1.1. *A problem is well-posed if [44]*

- *There exists a solution to the problem.*
- *The solution to the problem is unique.*
- *The solution depends continuously on data of the problem.*

A closely related concept is stability, we use the following initial-boundary-value problem to illustrate the definition of stability:

$$\begin{aligned}\frac{\partial \mathcal{U}}{\partial t} + \mathcal{D}(\mathcal{U}) &= \mathcal{F}, \quad x \in \Omega = [x_L, x_R], \quad t \geq 0, \\ \mathcal{B}(\mathcal{U}) &= \mathcal{G}(t), \quad x \in \Gamma, \\ \mathcal{I}(\mathcal{U}) &= \mathcal{N}(x), \quad t = 0.\end{aligned}\tag{2.1}$$

where $\mathcal{U}$ is a function of x and time t , $\mathcal{D}$ is a differential operator, $\mathcal{F}$ is a forcing term, $\mathcal{B}$ and $\mathcal{I}$ are the boundary operator and initial operator, respectively, where Γ is the boundary of the domain Ω . A problem is said to be stable if there exists a bound on the solution in terms of the data of the problem [43], i.e.,

$$\|\mathcal{U}\|^2 \leq C(\|\mathcal{G}\|_b^2 + \|\mathcal{N}\|_i^2 + \|\mathcal{F}\|_f^2), \quad (2.2)$$

where C is a constant independent of data and the subscripts represent potentially different norms. Stability is a necessary but insufficient condition for continuous dependence on the data of the problem. However, for linear problems, stability implies both continuous dependence on the data and uniqueness [43].

Theorem 2.1.1. *For linear problems, stability implies continuous dependence on the data and uniqueness.*

Proof. In order to prove the statement, we need to consider the following perturbed problem of (2.1) and let $\mathcal{V}$ be the solution to the perturbed problem,

$$\begin{aligned} \frac{\partial \mathcal{V}}{\partial t} + \mathcal{D}(\mathcal{V}) &= \mathcal{F} + \delta \mathcal{F} := \mathcal{F}', \quad x \in \Omega = [x_L, x_R], \quad t \geq 0 \\ \mathcal{B}(\mathcal{V}) &= \mathcal{G} + \delta \mathcal{G} := \mathcal{G}', \quad x \in \Gamma, \\ \mathcal{I}(\mathcal{V}) &= \mathcal{N} + \delta \mathcal{N} := \mathcal{N}', \quad t = 0. \end{aligned} \quad (2.3)$$

Then, let $\mathcal{W} := \mathcal{V} - \mathcal{U}$, assume $\mathcal{B}$ and $\mathcal{D}$ are linear operators, we subtract (2.1) from (2.3) to obtain

$$\begin{aligned} \frac{\partial \mathcal{W}}{\partial t} + \mathcal{D}(\mathcal{W}) &= \delta \mathcal{F}, \quad x \in \Omega = [x_L, x_R], \quad t \geq 0 \\ \mathcal{B}(\mathcal{W}) &= \delta \mathcal{G}, \quad x \in \Gamma, \\ \mathcal{I}(\mathcal{W}) &= \delta \mathcal{N}, \quad t = 0. \end{aligned} \quad (2.4)$$

If the problem (2.1) is stable, then the energy estimate (2.2) holds for (2.4), and therefore we obtain

$$\|\mathcal{W}\|^2 \leq C(\|\delta \mathcal{G}\|_b^2 + \|\delta \mathcal{N}\|_i^2 + \|\delta \mathcal{F}\|_f^2), \quad (2.5)$$

where small perturbation in the data $\delta \mathcal{G}, \delta \mathcal{N}, \delta \mathcal{F}$ result in small perturbation in $\mathcal{W}$. This is equivalent to say the solution to the problem (2.1) depends continuously on data of the problem. Note that $\delta = 0$ implies that $\mathcal{U} = \mathcal{V}$, which means the solution to the problem (2.1) is unique. $\square$

In this thesis, we will construct semi-discrete schemes that follow the continuous stability analysis in a one-to-one manner. In the remainder of this chapter, we illustrate the type of stability analysis that will later be used on the KZK equations by examining the stability analysis of the following: linear advection equation, linear diffusion equation, and inviscid Burgers' equation.

2.2 Continuous Stability Analysis of the Linear Advection Equation

We start by considering the following linear advection problem:

$$\begin{aligned}\frac{\partial \mathcal{U}}{\partial t} + a \frac{\partial \mathcal{U}}{\partial x} &= 0, \quad x \in [x_L, x_R], \quad t \in [0, T], \quad a > 0, \\ \mathcal{U}(x_L, t) &= \mathcal{G}(t), \\ \mathcal{U}(x, 0) &= \mathcal{I}(x),\end{aligned}\tag{2.6}$$

where $\mathcal{G}(t)$ and $\mathcal{I}(x)$ are the left boundary condition and initial condition, respectively, and T is the final time. To prove stability, we multiply (2.6) by $\mathcal{U}$ and then integrate over x to obtain

$$\int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{U}}{\partial t} dx + a \int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{U}}{\partial x} dx = 0.\tag{2.7}$$

Then, using integration by parts for the second term of (2.7), we have

$$\int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{U}}{\partial t} dx + \frac{1}{2} a \mathcal{U}^2 \Big|_{x_L}^{x_R} = 0.\tag{2.8}$$

Then, chain rule is applied to the first term to obtain

$$\frac{1}{2} \frac{d}{dt} \int_{x_L}^{x_R} \mathcal{U}^2 dx + \frac{1}{2} a \mathcal{U}^2 \Big|_{x_L}^{x_R} = 0.\tag{2.9}$$

Eq. (2.9) can be simplified by inserting the boundary condition. Doing so and after rearranging results in

$$\frac{1}{2} \frac{d}{dt} \int_{x_L}^{x_R} \mathcal{U}^2 dx = -a(\mathcal{U}(x_R, t)^2 - \mathcal{G}^2(t)) \leq a \mathcal{G}^2(t).\tag{2.10}$$

Denote the L_2 norm by $||\mathcal{U}|| := \sqrt{\int_{x_L}^{x_R} \mathcal{U}^2 dx}$, integrating (2.10) in time, and inserting the initial condition, we obtain

$$||\mathcal{U}(\cdot, T)||^2 \leq ||\mathcal{I}(\cdot)||^2 + a \int_0^T \mathcal{G}(t)^2 dt. \quad (2.11)$$

Eq. (2.11) shows that the L_2 norm of the solution is bounded by data of the problem, which indicates that the problem is stable. Since the problem (2.6) is linear, the solution to the problem is unique and continuously dependent on the data of the problem according to Theorem 2.1.1. Note that for periodic boundary conditions the above analysis reduces to the following stability estimate:

$$||\mathcal{U}(T)||^2 = ||\mathcal{I}(\cdot)||^2, \quad (2.12)$$

which means the energy remains constant.

2.3 Continuous Stability Analysis of the Linear Diffusion Equation

Consider the following diffusion equation with a homogeneous Neumann boundary condition and Dirichlet boundary condition on the left and right boundaries, respectively:

$$\begin{aligned} \frac{\partial \mathcal{U}}{\partial t} - \frac{\partial^2 \mathcal{U}}{\partial x^2} &= 0, \quad x \in [x_L, x_R], \quad t \in [0, T], \\ \frac{\partial \mathcal{U}}{\partial x}(x_L, t) &= 0, \quad \mathcal{U}(x_R, t) = 0, \\ \mathcal{U}(x, 0) &= \mathcal{I}(x). \end{aligned} \quad (2.13)$$

To prove stability, we first multiply by $\mathcal{U}$ and then integrate in x to obtain

$$\int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{U}}{\partial t} - \mathcal{U} \frac{\partial^2 \mathcal{U}}{\partial x^2} dx = 0. \quad (2.14)$$

Then, using integration by parts and applying Leibniz' rule, we have

$$\frac{1}{2} \frac{d}{dt} \int_{x_L}^{x_R} \mathcal{U}^2 dx - \mathcal{U} \frac{\partial \mathcal{U}}{\partial x} \Big|_{x_L}^{x_R} + \int_{x_L}^{x_R} \left(\frac{\partial \mathcal{U}}{\partial x} \right)^2 dx = 0. \quad (2.15)$$

Applying the boundary conditions to (2.15) and rearranging, results in

$$\frac{1}{2} \frac{d}{dt} \int_{x_L}^{x_R} \mathcal{U}^2 dx = - \int_{x_L}^{x_R} \left(\frac{\partial \mathcal{U}}{\partial x} \right)^2 dx. \quad (2.16)$$

Since the RHS of (2.15) is non-positive, we obtain the following inequality:

$$\frac{d}{dt} \int_{x_L}^{x_R} \mathcal{U}^2 dx \leq 0. \quad (2.17)$$

Finally, integrating (2.17) in time and applying the initial condition results in

$$\|\mathcal{U}(T)\|^2 \leq \|\mathcal{I}\|^2. \quad (2.18)$$

This demonstrates that the L_2 norm of the solution is bounded by the data of the problem and therefore, the problem 2.13 is stable.

2.4 Continuous Stability Analysis of the Inviscid Burgers' Equation

Consider the inviscid Burgers' equation:

$$\begin{aligned} \frac{\partial \mathcal{U}}{\partial t} + \mathcal{U} \frac{\partial \mathcal{U}}{\partial x} &= 0, \quad x \in [x_L, x_R], \quad t \in [0, T], \\ \mathcal{U}(x_L, t) &= 0, \quad \mathcal{U}(x_R, t) = 0, \\ \mathcal{U}(x, 0) &= \mathcal{I}(x), \end{aligned} \quad (2.19)$$

where $\mathcal{I}(x)$ is the initial condition. To prove stability, we multiply (2.19) by $\mathcal{U}$ and then integrate over x to obtain

$$\int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{U}}{\partial t} dx + \int_{x_L}^{x_R} \mathcal{U}^2 \frac{\partial \mathcal{U}}{\partial x} dx = 0. \quad (2.20)$$

Using integration by parts on the second term of (2.20), we obtain

$$\int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{U}}{\partial t} dx + \frac{1}{3} \mathcal{U}^3 \Big|_{x_L}^{x_R} = 0. \quad (2.21)$$

Then, boundary conditions can be applied to the (2.21), resulting in

$$\int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{U}}{\partial t} dx = 0. \quad (2.22)$$

Using chain rule on (2.22), we have

$$\frac{1}{2} \frac{d}{dt} \int_0^L \mathcal{U}^2 dx = 0. \quad (2.23)$$

Then, integrating (2.23) in time and applying the initial condition gives

$$\|\mathcal{U}(T)\|^2 = \|\mathcal{I}(0)\|^2. \quad (2.24)$$

Therefore, problem (2.19) is stable based on the given boundary and initial conditions.

In the upcoming chapter, we will develop discretizations for the simple PDEs discussed in this chapter, which enable us to follow the continuous stability analysis in a one-to-one sense. Semi-discrete stability analysis ensures that the solution to the semi-discrete form of the PDE remains bounded and does not blow up. Moreover, a consistent and stable scheme, as proven by the Lax-Richtmyer theorem, ensures convergence [81] for linear problems. Therefore, semi-discrete stability analysis plays a crucial role in these discretizations. The SBP-SAT technique is used to obtain the semi-discrete form of PDEs that are stable at the semi-discrete level.

Chapter 3

Summation-by-Parts methods

In this chapter, we introduce the basic definition and motivation for SBP operators and how these operators mimic integration by parts at the discrete level. Then, we show how to construct SBP operators using the CG approach. Finally, we demonstrate how to use SBP operators and SATs for the weak imposition of boundary conditions, to discretize the linear advection equation, linear diffusion equation, and Burgers' equation, and prove that the resulting semi-discrete forms are stable.

3.1 Basic Definition and Properties of SBP Operators

We first define $f_i := \mathcal{F}(x_i)$ for any function $\mathcal{F}$, where x_i is the i^{th} node in a one dimensional mesh. With this definition, $\mathbf{u} := [u_1, u_2, \dots, u_n]^T$ is a vector (grid function) containing the function $\mathcal{U}$ evaluated at nodes of a one-dimensional mesh having n nodes. SBP operators are matrix difference operators, that is, matrices that when applied to grid functions approximate derivatives at the mesh nodes. For example, given a function $\mathcal{U}$ and its associated grid function $\mathbf{u}$ on a one-dimensional mesh with n nodes, a matrix difference operator $\bar{D}_x \in \mathbb{R}^{n \times n}$ approximates the derivative in the following sense:

$$\bar{D}_x \mathbf{u} \approx \left[\left(\frac{\partial \mathcal{U}}{\partial x} \right)_1, \left(\frac{\partial \mathcal{U}}{\partial x} \right)_2, \dots, \left(\frac{\partial \mathcal{U}}{\partial x} \right)_n \right]^T. \quad (3.1)$$

SBP operators are matrix difference operators that satisfy certain properties. Specifically, they are defined as follows [25]:

Definition 3.1.1. *A matrix difference operator $\bar{D}_x \in \mathbb{R}^{n \times n}$ approximating the first derivative on the nodes $\mathbf{x} := [x_1, \dots, x_n]^T$ is a degree p SBP operator if*

1. $\bar{D}_x \mathbf{x}^k = k \mathbf{x}^{k-1}$, for $k = 0, 1, 2, \dots, p$
2. $\bar{D}_x := \bar{P}_x^{-1} \bar{Q}_x$, $\bar{P}_x = \bar{P}_x^T$, $\bar{P}_x > 0$
3. $\bar{Q}_x + \bar{Q}_x^T := \bar{E}_x := \mathbf{t}_R \mathbf{t}_R^T - \mathbf{t}_L \mathbf{t}_L^T = \text{diag}[-1, 0, \dots, 0, 1]$

One can show that definition 3.1.1, leads to $\bar{D}_x$ that approximate the first derivative with a truncation error of order p , i.e.,

$$\bar{D}_x \mathbf{f} = \frac{\partial \mathcal{F}}{\partial x}(\mathbf{x}) + \mathbf{e}_p, \quad (3.2)$$

where $\bar{D}_x \mathbf{f}$ is a vector of the derivative of $\mathcal{F}$ evaluated at the nodes $\mathbf{x}$ and $\max(|\mathbf{e}_p|) = O(\Delta x^p)$, where Δx is some measure of mesh spacing. Moreover, $\bar{P}_x$ is a symmetric positive definite matrix that approximates the L_2 inner product, that is

$$\mathbf{v}^T \bar{P}_x \mathbf{u} \approx \int_{x_L}^{x_R} \mathcal{V} \mathcal{U} dx. \quad (3.3)$$

Thus, we can show that $\bar{Q}_x$ approximates the following integral:

$$\mathbf{v}^T \bar{P}_x \bar{D}_x \mathbf{u} = \mathbf{v}^T \bar{Q}_x \mathbf{u} \approx \int_{x_R}^{x_L} \mathcal{V} \frac{\partial \mathcal{U}}{\partial x} dx. \quad (3.4)$$

In general, the norm matrix $\bar{P}_x$ is used to define inner product and norm as follows:

$$(\mathbf{u}, \mathbf{v})_P := \mathbf{u}^T \bar{P}_x \mathbf{v}, \quad (3.5)$$

$$\|\mathbf{u}, \mathbf{u}\|_P^2 := \mathbf{u}^T \bar{P}_x \mathbf{u}. \quad (3.6)$$

In this thesis, we will only consider diagonal norm $\bar{P}_x$. In this case, the diagonal entries of $\bar{P}_x$ are strictly positive and define a quadrature rule [25]. By taking advantage of SBP operators, we can not only discretize the equations, but also mimic integration by parts at the discrete level, which is what will enable the construction of schemes that have a one-to-one correspondence between continuous and semi-discrete stability proofs. To demonstrate that SBP operators mimic integration by parts, first, recall the integration by parts formula in one-dimension

$$\int_{x_L}^{x_R} \mathcal{V} \frac{\partial \mathcal{U}}{\partial x} dx + \int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} dx = \mathcal{V}(x_R) \mathcal{U}(x_R) - \mathcal{V}(x_L) \mathcal{U}(x_L). \quad (3.7)$$

Now we use our SBP operators to discretize the left hand side (LHS) of (3.7) as follows: $\mathbf{v}^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \mathbf{u} \approx \int_{x_L}^{x_R} \mathcal{V} \frac{\partial \mathcal{U}}{\partial x} dx$ and $\mathbf{u}^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \mathbf{v} \approx \int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} dx$. Hence, discretizing the LHS of (3.7) result in

$$\begin{aligned}
\mathbf{v}^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \mathbf{u} + \mathbf{u}^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \mathbf{v} &= \mathbf{v}^T \bar{\mathbf{Q}}_x \mathbf{u} + \mathbf{u}^T \bar{\mathbf{Q}}_x \mathbf{v} \\
&= \mathbf{v}^T \bar{\mathbf{Q}}_x \mathbf{u} + (\mathbf{v}^T \bar{\mathbf{Q}}_x^T \mathbf{u})^T \\
&= \mathbf{v}^T \bar{\mathbf{Q}}_x \mathbf{u} + \mathbf{v}^T \bar{\mathbf{Q}}_x^T \mathbf{u} \\
&= \mathbf{v}^T (\bar{\mathbf{Q}}_x + \bar{\mathbf{Q}}_x^T) \mathbf{u} \\
&= \mathbf{v}^T \bar{\mathbf{E}}_x \mathbf{u} \\
&= \mathbf{v}_n \mathbf{u}_n - \mathbf{v}_1 \mathbf{u}_1.
\end{aligned} \tag{3.8}$$

which mimics integration by parts term by term.

For the KZK equations we will require the approximation of second derivatives and are similarly interested in discretizations that mimic integration by parts for such terms. First, we will construct an approximation of the second derivative constructed by applying the first derivative twice. Later in the thesis we will present a more general treatment of the second derivative.

Theorem 3.1.1. *Assume that $\bar{\mathbf{D}}_x, \bar{\mathbf{P}}_x, \bar{\mathbf{Q}}_x, \bar{\mathbf{E}}_x$ are the constituent matrices of an SBP operator as per Definition 3.1.1, then the second derivative operator can be constructed as*

$$\bar{\mathbf{D}}_x \bar{\mathbf{D}}_x = \bar{\mathbf{P}}_x^{-1} (-\bar{\mathbf{D}}_x^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x + \bar{\mathbf{E}}_x \bar{\mathbf{D}}_x). \tag{3.9}$$

Proof. According to the definition 3.1.1, we have that $\bar{\mathbf{D}}_x = \bar{\mathbf{P}}_x^{-1} \bar{\mathbf{Q}}_x$ and $\bar{\mathbf{Q}}_x^T = \bar{\mathbf{E}}_x - \bar{\mathbf{Q}}_x$, then

$$\bar{\mathbf{D}}_x \bar{\mathbf{D}}_x = \bar{\mathbf{P}}_x^{-1} \bar{\mathbf{Q}}_x \bar{\mathbf{D}}_x = \bar{\mathbf{P}}_x^{-1} (\bar{\mathbf{E}}_x - \bar{\mathbf{Q}}_x^T) \bar{\mathbf{D}}_x = \bar{\mathbf{P}}_x^{-1} (-\bar{\mathbf{Q}}_x^T \bar{\mathbf{D}}_x + \bar{\mathbf{E}}_x \bar{\mathbf{D}}_x). \tag{3.10}$$

Next, we use the identity $\bar{\mathbf{P}}_x^{-1} \bar{\mathbf{P}}_x = \bar{\mathbf{I}}$, where $\bar{\mathbf{I}}$ is an $n \times n$ identity matrix, and the SBP property $\bar{\mathbf{D}}_x = \bar{\mathbf{P}}_x^{-1} \bar{\mathbf{Q}}_x$ transforming (3.10) as

$$\bar{\mathbf{D}}_x \bar{\mathbf{D}}_x = \bar{\mathbf{P}}_x^{-1} (-\bar{\mathbf{Q}}_x^T \bar{\mathbf{P}}_x^{-1} \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x + \bar{\mathbf{E}}_x \bar{\mathbf{D}}_x) = \bar{\mathbf{P}}_x^{-1} (-\bar{\mathbf{D}}_x^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x + \bar{\mathbf{E}}_x \bar{\mathbf{D}}_x) \tag{3.11}$$

as desired. $\square$

Next, we demonstrate that the application of the first derivative twice results in a discrete operator that mimics integration by parts. To show this, recall the integration by

parts for the second derivative term is

$$\int_{x_L}^{x_R} \mathcal{V} \frac{\partial^2 \mathcal{U}}{\partial x^2} dx + \int_{x_L}^{x_R} \frac{\partial \mathcal{V}}{\partial x} \frac{\partial \mathcal{U}}{\partial x} dx = \mathcal{V}(x_R) \frac{\partial \mathcal{U}}{\partial x}(x_R) - \mathcal{V}(x_L) \frac{\partial \mathcal{U}}{\partial x}(x_L). \quad (3.12)$$

The LHS of (3.12) can be discretized by using SBP operators as follows:

$\mathbf{v}^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \bar{\mathbf{D}}_x \mathbf{u} \approx \int_{x_L}^{x_R} \mathcal{V} \frac{\partial^2 \mathcal{U}}{\partial x^2} dx$ and $\mathbf{v}^T \bar{\mathbf{D}}_x^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \mathbf{u} \approx \int_{x_L}^{x_R} \frac{\partial \mathcal{V}}{\partial x} \frac{\partial \mathcal{U}}{\partial x} dx$. Hence, discretizing the LHS of (3.12) gives

$$\begin{aligned} \mathbf{v}^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \bar{\mathbf{D}}_x \mathbf{u} + \mathbf{v}^T \bar{\mathbf{D}}_x^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \mathbf{u} &= \mathbf{v}^T (\bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \bar{\mathbf{D}}_x + \bar{\mathbf{D}}_x^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x) \mathbf{u} \\ &= \mathbf{v}^T (-\bar{\mathbf{D}}_x^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x + \bar{\mathbf{E}}_x \bar{\mathbf{D}}_x + \bar{\mathbf{D}}_x^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x) \mathbf{u} \\ &= \mathbf{v}^T \bar{\mathbf{E}}_x \bar{\mathbf{D}}_x \mathbf{u}, \end{aligned} \quad (3.13)$$

which mimics integration by parts.

In this thesis, we construct SBP operators by first constructing them in a fixed computational coordinate system and then using a linear mapping to construct SBP operators in physical space. To demonstrate the approach, consider a linear mapping between the computational domain $\xi \in [-1, 1]$ and the physical domain $x \in [x_L, x_R]$. The linear mapping between the computational domain $\xi \in [-1, 1]$ and the physical domain $x \in [x_L, x_R]$ is given by

$$a\xi + b = x, \quad (3.14)$$

then we have that

$$x = \frac{(x_R - x_L)\xi}{2} + \frac{x_R + x_L}{2}, \quad (3.15)$$

and

$$\frac{\partial \xi}{\partial x} = \frac{2}{x_R - x_L}. \quad (3.16)$$

Then, according to the (3.15) and using chain rule, we have that

$$\begin{aligned} \bar{\mathbf{D}}_x &= \frac{\partial \xi}{\partial x} \bar{\mathbf{D}}_\xi = \frac{2}{x_R - x_L} \bar{\mathbf{D}}_\xi, \\ \bar{\mathbf{P}}_x &= \frac{\partial x}{\partial \xi} \bar{\mathbf{P}}_\xi = \frac{x_R - x_L}{2} \bar{\mathbf{P}}_\xi. \end{aligned} \quad (3.17)$$

Therefore, taking advantage of this approach, instead of computing the SBP operators for each new domain, we only need to compute the SBP operator in computational space once, store it and then use it to construct operators for physical coordinates via (3.17). In the following, we will concentrate on the construction of SBP operators for the computational domain. Specifically, we will consider SBP operators constructed on Gauss-Lobatto (GL) nodes that are extended to the full mesh via the CG approach [46, 47].

3.2 Continuous Galerkin SBP operators

In this subsection, we will illustrate how to construct CG-SBP operators from local element operators that are defined in the computational domain. The local SBP operators are generated by using Lagrange interpolation basis. We first recall the definition of Lagrange basis as following.

Definition 3.2.1. *Suppose we have n distinct nodes $\xi_1, \xi_2, \dots, \xi_n$, then the degree $n - 1$ Lagrange basis is the set $\mathcal{L}_1(\xi), \mathcal{L}_2(\xi), \dots, \mathcal{L}_n(\xi)$ that satisfy $\mathcal{L}_j(\xi_m) = 0$ if $j \neq m$ and $\mathcal{L}_j(\xi_j) = 1$, where $1 \leq m, j \leq n$. Each basis polynomial can be explicitly described by the product:*

$$\mathcal{L}_j(\xi) = \prod_{\substack{1 \leq m \leq n \\ m \neq j}}^n \frac{\xi - \xi_m}{\xi_j - \xi_m}. \quad (3.18)$$

With these interpolating polynomials, we can construct an approximation to a function that interpolates through a set of nodes in computational coordinates as

$$\mathcal{U}(\xi) \approx \mathcal{U}_h(\xi) := \sum_{i=1}^n u_i \mathcal{L}_i(\xi), \quad (3.19)$$

where we will consider nodes that are distributed as $-1 \leq \xi_1 < \dots < \xi_n \leq 1$. In this thesis, the GL nodes are used in computational space on each element to construct CG-SBP operators.

To construct the element-wise SBP operators in computational space, we start by determining the structure of diagonal mass matrix $\bar{\mathbf{P}}_\xi$, and then construct $\bar{\mathbf{D}}_\xi, \bar{\mathbf{Q}}_\xi, \bar{\mathbf{M}}_\xi$ based on the same idea. The matrix $\bar{\mathbf{M}}_\xi$ will be used in the discretization of the KZK equations and will be used to approximate the following type of integral terms:

$$\partial_x^{-1} \mathcal{F}(x) := \int_{x_L}^x \mathcal{F}(s) ds. \quad (3.20)$$

For the purpose of constructing $\bar{\mathbf{P}}_\xi$, consider the function $\mathcal{F}(\xi)$, then using the polynomial approximation 3.19, we obtain

$$\int_{-1}^1 \mathcal{F}(\xi) d\xi \approx \int_{-1}^1 \sum_{j=1}^n \mathcal{F}(\xi_j) \mathcal{L}_j(\xi) d\xi = \sum_{j=1}^n \mathcal{F}(\xi_j) w_j, \quad (3.21)$$

where $w_j := \int_{-1}^1 \mathcal{L}_j(\xi) d\xi$ and define a set of quadrature weights. Then, the diagonal mass matrix $\bar{\mathbf{P}}_\xi := \text{diag}([w_1, \dots, w_n])$, which defines an approximation to the L_2 inner product, since

$$\int_{-1}^1 \mathcal{U} \mathcal{V} d\xi \approx \sum_{j=1}^n \int_{-1}^1 \mathcal{U}(\xi_j) \mathcal{V}(\xi_j) \mathcal{L}_j(\xi) d\xi = \sum_{j=1}^n \mathcal{U}(\xi_j) \mathcal{V}(\xi_j) w_j = \mathbf{u}^T \bar{\mathbf{P}}_\xi \mathbf{v}. \quad (3.22)$$

Similarly, in order to construct $\bar{\mathbf{D}}_\xi$, $\bar{\mathbf{Q}}_\xi$ and $\bar{\mathbf{M}}_\xi$, consider the following:

$$\frac{d\mathcal{U}(\xi)}{d\xi} \approx \sum_{i=1}^n \mathcal{U}(\xi_i) \frac{d\mathcal{L}_i(\xi)}{d\xi}, \quad (3.23)$$

$$\int_{-1}^1 \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} d\xi \approx \sum_{i=1}^n \sum_{j=1}^n \mathcal{U}(\xi_i) \mathcal{V}(\xi_j) \int_{-1}^1 \mathcal{L}_i(\xi) \frac{d\mathcal{L}_j(\xi)}{d\xi} d\xi, \quad (3.24)$$

$$\int_{-1}^\xi \mathcal{U} d\xi \approx \sum_{j=1}^n \mathcal{U}(\xi_j) \int_{-1}^\xi \mathcal{L}_j(\xi) d\xi. \quad (3.25)$$

Thus, one dimensional SBP operators on each element, in computational space, can be construct, based on equation (3.22), (3.23), (3.24) and (3.25), as

$$\bar{\mathbf{P}}_\xi(i, i) = \int_{\xi_L}^{\xi_R} \mathcal{L}_i d\xi, \quad (3.26)$$

and the $(i, j)^{th}$ entries of $\bar{\mathbf{D}}_\xi$, $\bar{\mathbf{Q}}_\xi$ and $\bar{\mathbf{M}}_\xi$ are defined as

$$\bar{\mathbf{D}}_\xi(i, j) = \frac{d\mathcal{L}_i(\xi_j)}{d\xi}, \quad (3.27)$$

$$\bar{\mathbf{Q}}_\xi(i, j) = \int_{\xi_L}^{\xi_R} \mathcal{L}_i \frac{\partial \mathcal{L}_j}{\partial \xi} d\xi, \quad (3.28)$$

$$\bar{\mathbf{M}}_\xi(i, j) = \int_{\xi_L}^{\xi_i} \mathcal{L}_j d\xi, \quad (3.29)$$

where ξ_i is the i^{th} node in the computational domain, and

$$\bar{\mathbf{M}}_\xi \mathbf{f} \approx \left[\int_{\xi_L}^{\xi_1} \mathcal{F}(s) ds, \int_{\xi_L}^{\xi_2} \mathcal{F}(s) ds, \dots, \int_{\xi_L}^{\xi_n} \mathcal{F}(s) ds \right]^T.$$

With this construction, we have that $\bar{\mathbf{E}}_\xi$ on an element can be constructed from the definition 3.1.1, where $\mathbf{t}_R = [\mathcal{L}_1(\xi_n), \dots, \mathcal{L}_n(\xi_n)]^T = [0, \dots, 0, 1]^T$, $\mathbf{t}_L = [\mathcal{L}_1(\xi_1), \dots, \mathcal{L}_n(\xi_1)]^T = [1, 0, \dots, 0]^T$ for the GL nodes. Next, we demonstrate that the resulting operators are SBP. First, consider the following equality:

$$\bar{\mathbf{Q}}_\xi(i, j) + \bar{\mathbf{Q}}_\xi(i, j)^T = \int_{\xi_L}^{\xi_R} \mathcal{L}_i \frac{\partial \mathcal{L}_j}{\partial \xi} d\xi + \int_{\xi_L}^{\xi_R} \mathcal{L}_j \frac{\partial \mathcal{L}_i}{\partial \xi} d\xi. \quad (3.30)$$

Using integration by parts we obtain

$$(\bar{\mathbf{Q}}_\xi + \bar{\mathbf{Q}}_\xi^T)(i, j) = \mathcal{L}_i \mathcal{L}_j|_{\xi_L}^{\xi_R}, \quad (3.31)$$

which indicates that

$$\bar{\mathbf{Q}}_\xi + \bar{\mathbf{Q}}_\xi^T = \mathbf{t}_R \mathbf{t}_R^T - \mathbf{t}_L \mathbf{t}_L^T = \bar{\mathbf{E}}_\xi. \quad (3.32)$$

Moreover, we need to show that $\bar{\mathbf{D}}_\xi \boldsymbol{\xi}^k = \bar{\mathbf{P}}_\xi^{-1} \bar{\mathbf{Q}}_\xi \boldsymbol{\xi}^k = k \boldsymbol{\xi}^{k-1}$ for $k = 0, 1, 2, \dots, p$. To prove these properties, we will make use of the Vandermonde matrix V defined as

$$V := \begin{bmatrix} 1 & (\xi_0)^1 & (\xi_0)^2 & \dots & (\xi_0)^p \\ 1 & (\xi_1)^1 & (\xi_1)^2 & \dots & (\xi_1)^p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & (\xi_n)^1 & (\xi_n)^2 & \dots & (\xi_n)^p \end{bmatrix}. \quad (3.33)$$

We also define V_ξ as

$$V_\xi := \begin{bmatrix} 0 & 1 & 2\xi_0 & \dots & p\xi_0^{p-1} \\ 0 & 1 & 2\xi_1 & \dots & p\xi_1^{p-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & 2\xi_n & \dots & p\xi_n^{p-1} \end{bmatrix}. \quad (3.34)$$

According to the (3.26) and (3.28), we obtain

$$(\boldsymbol{\xi}^i)^T \bar{\mathbf{Q}}_\xi \boldsymbol{\xi}^j = \int \boldsymbol{\xi}^i \frac{\partial \boldsymbol{\xi}^j}{\partial \xi} d\xi = (\boldsymbol{\xi}^i)^T \bar{\mathbf{P}}_\xi \frac{\partial \boldsymbol{\xi}^j}{\partial \xi}; \quad (3.35)$$

note that the above equality results because the quadrature rule on the GL nodes is degree $2p - 1$ [24]. Then, considering (3.35) for $i, j = 0, 1, \dots, p$, we obtain the following:

$$V^T \bar{\mathbf{Q}}_\xi V = V^T \bar{\mathbf{P}}_\xi V_\xi. \quad (3.36)$$

Since the Vandermonde matrix V is invertible if and only if ξ_i are distinct and $n = p + 1$ [89, 62], which is the case considered here, we obtain

$$\bar{\mathbf{Q}}_\xi V = \bar{\mathbf{P}}_\xi V_\xi. \quad (3.37)$$

Since the $\bar{\mathbf{P}}_\xi$ is invertible (this is immediate since it is diagonal with positive entries), then (3.37) can be rewritten as

$$\bar{\mathbf{D}}_\xi V = \bar{\mathbf{P}}_\xi^{-1} \bar{\mathbf{Q}}_\xi V = V_\xi, \quad (3.38)$$

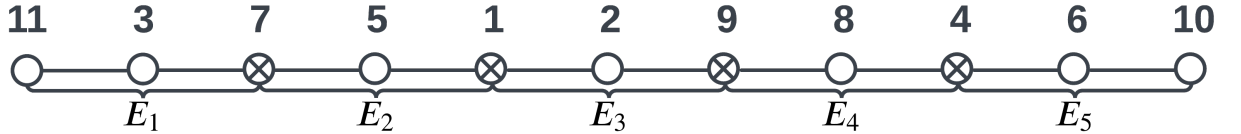
which indicates that

$$\bar{\mathbf{D}}_\xi \boldsymbol{\xi}^k = k \boldsymbol{\xi}^{k-1}, \quad k = 0, 1, \dots, p. \quad (3.39)$$

Therefore, these operators satisfy the definition of an SBP operator.

Next, we will construct global one-dimensional CG operators by combining the local SBP operators into a global operator. For this purpose, suppose we have N elements each having n nodes, where elements touch at a common interface; thus, overall there are $l = nN - (N - 1)$ nodes. In order to combine the local operators into a global operators we introduce the mapping matrices $\mathbf{R}_e$ that map $\mathbf{u}_g$ to $\mathbf{u}_e$, i.e. $\mathbf{R}_e \mathbf{u}_g = \mathbf{u}_e$, where $\mathbf{u}_g$ is $\mathcal{U}$ evaluated at global nodes and $\mathbf{u}_e$ is $\mathcal{U}$ evaluated at local nodes for element e . $\mathbf{R}_e$ is a matrix of size $n \times l$ for element e , where $e = 1, 2, \dots, N$. The entries (i, j) of $\mathbf{R}_e$ are 1 for a node that is the i^{th} node in local coordinates and the j^{th} node in global coordinates, where the remaining entries of $\mathbf{R}_e$ are zero. We illustrate the mapping matrix through the following example:

Example 3.2.1. Suppose there are 5 element, namely E_1, E_2, E_3, E_4 and E_5 , with 3 nodes for each element, indicating that we have the 11 nodes in total and are labeled as in the diagram below. The common nodes are denoted as $\otimes$. Based on how we define $\mathbf{R}_e$, we have that $\mathbf{R}_1 \mathbf{u}_g = \mathbf{u}_1$, $\mathbf{R}_2 \mathbf{u}_g = \mathbf{u}_2$, $\mathbf{R}_3 \mathbf{u}_g = \mathbf{u}_3$, $\mathbf{R}_4 \mathbf{u}_g = \mathbf{u}_4$, $\mathbf{R}_5 \mathbf{u}_g = \mathbf{u}_5$ where



$$\mathbf{R}_1 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}, \mathbf{R}_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{R}_3 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}, \mathbf{R}_4 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{R}_5 = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix},$$

$$\mathbf{u}_1 = \begin{bmatrix} u_{11} \\ u_3 \\ u_7 \end{bmatrix}, \mathbf{u}_2 = \begin{bmatrix} u_7 \\ u_5 \\ u_1 \end{bmatrix}, \mathbf{u}_3 = \begin{bmatrix} u_1 \\ u_2 \\ u_9 \end{bmatrix}, \mathbf{u}_3 = \begin{bmatrix} u_9 \\ u_8 \\ u_4 \end{bmatrix}, \mathbf{u}_4 = \begin{bmatrix} u_4 \\ u_6 \\ u_{10} \end{bmatrix},$$

and $\mathbf{u}_g = [u_1, u_2, u_3, u_4, u_5, u_6, u_7, u_8, u_9, u_{10}, u_{11}]$.

We now have all the necessary components to construct the one-dimensional CG-SBP operators.

Definition 3.2.2. *The one dimensional CG SBP operators $\bar{\mathbf{P}}_{xg}$, $\bar{\mathbf{Q}}_{xg}$ and $\bar{\mathbf{E}}_{xg}$, are defined as*

$$\bar{\mathbf{P}}_{xg} := \sum_{i=1}^N \mathbf{R}_i^T \bar{\mathbf{P}}_x \mathbf{R}_i, \quad (3.40)$$

$$\bar{\mathbf{Q}}_{xg} := \sum_{i=1}^N \mathbf{R}_i^T \bar{\mathbf{Q}}_x \mathbf{R}_i, \quad (3.41)$$

$$\bar{\mathbf{E}}_{xg} := \sum_{i=1}^N \mathbf{R}_i^T \bar{\mathbf{E}}_x \mathbf{R}_i. \quad (3.42)$$

Note that we use the SBP operators for the computational domain and the linear mapping to construct the local physical coordinate operators.

Hence, we can construct a one-dimensional SBP differentiation matrix over the mesh as $\bar{\mathbf{D}}_{xg} = \bar{\mathbf{P}}_{xg}^{-1} \bar{\mathbf{Q}}_{xg}$. The proof that this operator is polynomially exact is the same as for the single element case, namely (3.35) - (3.39).

What remains, is to show that these global matrices also mimic integration by parts, that is, they are SBP. First note that

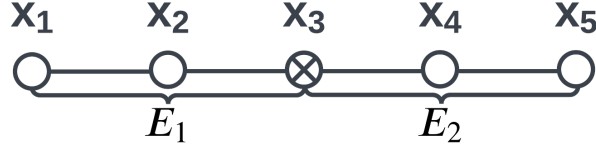
$$\bar{\mathbf{Q}}_{xg} + \bar{\mathbf{Q}}_{xg}^T = \sum_{i=1}^N \mathbf{R}_i^T \bar{\mathbf{Q}}_x \mathbf{R}_i + \mathbf{R}_i^T \bar{\mathbf{Q}}_x^T \mathbf{R}_i = \sum_{i=1}^N \mathbf{R}_i^T \bar{\mathbf{E}}_x \mathbf{R}_i = \bar{\mathbf{E}}_{xg}, \quad (3.43)$$

then we have

$$\mathbf{u}_g^T \bar{\mathbf{Q}}_{xg} \mathbf{v}_g + \mathbf{v}_g^T \bar{\mathbf{Q}}_{xg} \mathbf{u}_g = \mathbf{v}_g^T \bar{\mathbf{E}}_{xg} \mathbf{u}_g = \mathbf{v}_g^T (\mathbf{t}_{Rg} \mathbf{t}_{Rg}^T - \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T) \mathbf{u}_g, \quad (3.44)$$

where $\mathbf{t}_{Lg} = [1, 0, \dots, 0]$ and $\mathbf{t}_{Rg} = [0, \dots, 0, 1]$. The last equality results from the fact that the nonzero contributions from the $\bar{\mathbf{E}}_x$ matrices originating from interior elements cancel out with the exception of the left contribution from the left element and the right contribution from the right element. Therefore, the CG operators satisfy the SBP properties. Next, we need to extend $\bar{\mathbf{M}}_\xi$ from a per element operator to a global operator. The following example motivates the construction of $\bar{\mathbf{M}}_{xg}$.

Example 3.2.2. Assume there are two elements and three nodes for each element as per the diagram below.



Note that $\bar{\mathbf{M}}_{xg} \mathbf{f}_g$ needs to return a vector such that the i^{th} entry is

$$(\bar{\mathbf{M}}_{xg} \mathbf{f}_g)_i \approx \int_{x_1}^{x_i} \mathcal{F}(s) ds. \quad (3.45)$$

For the setup above, we approximate $\mathcal{F}$ on each element as

$$\mathcal{F}_h^{(1)} = \sum_{i=1}^3 f_i^{(1)} \mathcal{L}_i^{(1)}(x), \quad \mathcal{F}_h^{(2)} = \sum_{i=1}^3 f_i^{(2)} \mathcal{L}_i^{(2)}(x), \quad \text{where } f_3^{(1)} = f_1^{(2)}.$$

Using these expansions we can approximate the integration to, for example, the fourth node as

$$\begin{aligned} \int_{x_1}^{x_4} \mathcal{F} dx &\approx \int_{x_1}^{x_4} \mathcal{F}_h^{(1)}(x) + \mathcal{F}_h^{(2)}(x) = \int_{x_1}^{x_3} \sum_{i=1}^3 f_i^{(1)} \mathcal{L}_i^{(1)} dx + \int_{x_3}^{x_4} \sum_{i=1}^3 f_i^{(2)} \mathcal{L}_i^{(2)} dx \\ &= \int_{x_1}^{x_3} f_1^{(1)} \mathcal{L}_1^{(1)} dx + \int_{x_1}^{x_3} f_2^{(1)} \mathcal{L}_2^{(1)} dx + \int_{x_1}^{x_3} f_3^{(1)} \mathcal{L}_3^{(1)} dx \\ &\quad + \int_{x_3}^{x_4} f_1^{(2)} \mathcal{L}_1^{(2)} dx + \int_{x_3}^{x_4} f_2^{(2)} \mathcal{L}_2^{(2)} dx + \int_{x_3}^{x_4} f_3^{(2)} \mathcal{L}_3^{(2)} dx \\ &= \int_{x_1}^{x_3} f_1 \mathcal{L}_1^{(1)} dx + \int_{x_1}^{x_3} f_2 \mathcal{L}_2^{(1)} dx + \int_{x_1}^{x_3} (\mathcal{L}_3^{(1)} + \mathcal{L}_1^{(2)}) f_3 dx \\ &\quad + \int_{x_3}^{x_4} f_4 \mathcal{L}_2^{(2)} dx + \int_{x_3}^{x_4} f_5 \mathcal{L}_3^{(2)} dx. \end{aligned}$$

Hence, in this case, we have

$$\overline{\mathbf{M}}_{xg} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ \int_{x_1}^{x_2} \mathcal{L}_1^{(1)} dx & \int_{x_1}^{x_2} \mathcal{L}_2^{(1)} dx & \int_{x_1}^{x_2} \mathcal{L}_3^{(1)} dx & 0 & 0 \\ \int_{x_1}^{x_3} \mathcal{L}_1^{(1)} dx & \int_{x_1}^{x_3} \mathcal{L}_2^{(1)} dx & \int_{x_1}^{x_3} \mathcal{L}_3^{(1)} dx & 0 & 0 \\ \int_{x_1}^{x_3} \mathcal{L}_1^{(1)} dx & \int_{x_1}^{x_3} \mathcal{L}_2^{(1)} dx & \int_{x_1}^{x_3} \mathcal{L}_3^{(1)} dx + \int_{x_3}^{x_4} \mathcal{L}_1^{(2)} dx & \int_{x_3}^{x_4} \mathcal{L}_2^{(2)} dx & \int_{x_3}^{x_4} \mathcal{L}_3^{(2)} dx \\ \int_{x_1}^{x_3} \mathcal{L}_1^{(1)} dx & \int_{x_1}^{x_3} \mathcal{L}_2^{(1)} dx & \int_{x_1}^{x_3} \mathcal{L}_3^{(1)} dx + \int_{x_3}^{x_5} \mathcal{L}_1^{(2)} dx & \int_{x_3}^{x_5} \mathcal{L}_2^{(2)} dx & \int_{x_3}^{x_5} \mathcal{L}_3^{(2)} dx \end{bmatrix}, \quad (3.46)$$

and it can be visualized as follows:

$$\overline{\mathbf{M}}_{xg} = \frac{x_R - x_L}{2} \begin{bmatrix} \overline{\mathbf{M}}_{\tilde{\xi}} & & & \\ \tilde{\mathbf{M}} & \overline{\mathbf{M}}_{\tilde{\xi}} & & \\ \tilde{\mathbf{M}} & \tilde{\mathbf{M}} & \overline{\mathbf{M}}_{\tilde{\xi}} & \\ \tilde{\mathbf{M}} & \tilde{\mathbf{M}} & \tilde{\mathbf{M}} & \overline{\mathbf{M}}_{\tilde{\xi}} \end{bmatrix},$$

where $\overline{\mathbf{M}}_{\tilde{\xi}}$ accumulates the targeted function for each element. Recalling $\overline{\mathbf{M}}_{\xi} \in \mathbb{R}^{n \times n}$ defined in (3.29), $\overline{\mathbf{M}}_{\tilde{\xi}}$ has the following general form:

$$\overline{\mathbf{M}}_{\tilde{\xi}} := \frac{\Delta \tilde{\xi}}{2} \overline{\mathbf{M}}_{\xi}, \quad (3.47)$$

where $\Delta \tilde{\xi}$ is the length of element on the computational domain. Then, $\tilde{\mathbf{M}} \in \mathbb{R}^{n \times n}$ is defined as

$$\tilde{\mathbf{M}} := \begin{bmatrix} \vec{0} \\ \overline{\mathbf{M}}_{\tilde{\xi}}(n, :) \\ \vdots \\ \overline{\mathbf{M}}_{\tilde{\xi}}(n, :) \end{bmatrix}. \quad (3.48)$$

Therefore, we can construct the global operator $\overline{\mathbf{M}}_{xg}$ based on the local operators by using the mapping matrices as follows:

$$\overline{\mathbf{M}}_{xg} = \frac{x_R - x_L}{2} \left(\sum_{i=1}^N \mathbf{R}_i^T \overline{\mathbf{M}}_{\tilde{\xi}} \mathbf{R}_i + \sum_{j=1}^N \sum_{k=j+1}^N \mathbf{R}_k^T \tilde{\mathbf{M}} \mathbf{R}_j \right). \quad (3.49)$$

Next, we need to consider how to construct the second derivative SBP operator globally. The definition of the second derivative operator is introduced as follows [66].

Definition 3.2.3. (*Second derivative operator*) The operator $\bar{D}_{2xg} := \bar{P}_{xg}^{-1}(-\bar{A}_{xg} + \bar{E}_{xg}\bar{D}_{xg})$ approximating $\frac{\partial^2}{\partial x^2}$ is a second derivative SBP operator if $\bar{A}_{xg} + \bar{A}_{xg}^T > 0$ and $\bar{A}_{xg}$ is a symmetric matrix, where $\bar{E}_{xg}$, $\bar{D}_{xg}$ and $\bar{P}_{xg}$ are one-dimensional global SBP operators defined in 3.2.2.

In this thesis, two options for $\bar{A}_{xg}$ are considered. We can choose $\bar{A}_{xg} = \sum_{i=1}^N R_i^T \bar{D}_x^T \bar{P}_x \bar{D}_x R_i$ or $\bar{A}_{xg} = \bar{D}_{xg}^T \bar{P}_{xg} \bar{D}_{xg}$. In the next section, we demonstrate how to discretize PDEs using these operators.

3.3 Simultaneous Approximation Term

In this thesis, we use the SAT technique to enforce the boundary conditions weakly, that is, our discretization only approximately satisfies the boundary conditions. In this section, we motivate the SATs that will later be used for the KZK equations by developing SATs for the linear advection equation, linear diffusion equation, and the Burgers' equation.

3.3.1 SBP-SAT Discretization of the Linear Advection Equation

We discretize the linear advection equation, in space, using CG-SBP operators and SATs as follows:

$$\frac{d\mathbf{u}}{dt} + a\bar{D}_{xg}\mathbf{u} = \sigma_1 a\bar{P}_{xg}^{-1}\mathbf{t}_{Lg}(\mathbf{t}_{Lg}^T\mathbf{u} - \mathbf{t}_{Rg}^T\mathbf{u}) + \sigma_2 a\bar{P}_{xg}^{-1}\mathbf{t}_{Rg}(\mathbf{t}_{Rg}^T\mathbf{u} - \mathbf{t}_{Lg}^T\mathbf{u}), \quad (3.50)$$

where the SATs are given as

$$\mathbf{SAT}_L := a\sigma_1\bar{P}_{xg}^{-1}\mathbf{t}_{Lg}(\mathbf{t}_{Lg}^T\mathbf{u} - \mathbf{t}_{Rg}^T\mathbf{u}), \quad \mathbf{SAT}_R := a\sigma_2\bar{P}_{xg}^{-1}\mathbf{t}_{Rg}(\mathbf{t}_{Rg}^T\mathbf{u} - \mathbf{t}_{Lg}^T\mathbf{u}), \quad (3.51)$$

and σ_1 and σ_2 are the parameters for the SATs that will be chosen so that the scheme is stable. The SATs impose the boundary conditions weakly, where $\mathbf{SAT}_L$ imposes the left periodic boundary condition and $\mathbf{SAT}_R$ imposes the right periodic boundary condition. To understand how the SATs encode the boundary conditions, note, for example, that $\mathbf{t}_{Lg}^T\mathbf{u} - \mathbf{t}_{Rg}^T\mathbf{u} \approx \mathcal{U}(x_L) - \mathcal{U}(x_R) = 0$. The LHS of (3.50) is the discretization of the linear advection equation using CG-SBP operators while the RHS of (3.50) are the SATs, which

imposed the periodic boundary condition weakly. We now prove stability at the semi-discrete level in exactly the same way as at the continuous level. The first step is to multiply by the solution and discretely integrate, this is accomplished by multiplying (3.50) by $\mathbf{u}^T \bar{\mathbf{P}}_{xg}$ and since $\bar{\mathbf{D}}_{xg} = \bar{\mathbf{P}}_{xg}^{-1} \bar{\mathbf{Q}}_{xg}$, then we have that

$$\mathbf{u}^T \bar{\mathbf{P}}_{xg} \frac{d\mathbf{u}}{dt} + a \mathbf{u}^T \bar{\mathbf{Q}}_{xg} \mathbf{u} = \sigma_1 a \mathbf{u}^T \mathbf{t}_{Lg} (\mathbf{t}_{Lg}^T \mathbf{u} - \mathbf{t}_{Rg}^T \mathbf{u}) + \sigma_2 a \mathbf{u}^T \mathbf{t}_{Rg} (\mathbf{t}_{Rg}^T \mathbf{u} - \mathbf{t}_{Lg}^T \mathbf{u}). \quad (3.52)$$

Using the fact that $\mathbf{u}^T \bar{\mathbf{Q}}_{xg} \mathbf{u} = \mathbf{u}^T \bar{\mathbf{Q}}_{xg}^T \mathbf{u}$, $\bar{\mathbf{Q}}_{xg} + \bar{\mathbf{Q}}_{xg}^T = \bar{\mathbf{E}}_{xg}$, and $\bar{\mathbf{E}}_{xg} = \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T - \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T$, then we can rewrite (3.52) as

$$\mathbf{u}^T \bar{\mathbf{P}}_{xg} \frac{d\mathbf{u}}{dt} + \frac{1}{2} a \mathbf{u}^T (\mathbf{t}_{Rg} \mathbf{t}_{Rg}^T - \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T) \mathbf{u} = \sigma_1 a \mathbf{u}^T \mathbf{t}_{Rg} (\mathbf{t}_{Rg}^T \mathbf{u} - \mathbf{t}_{Lg}^T \mathbf{u}) + \sigma_2 a \mathbf{u}^T \mathbf{t}_{Lg} (\mathbf{t}_{Lg}^T \mathbf{u} - \mathbf{t}_{Rg}^T \mathbf{u}). \quad (3.53)$$

Combining common terms in (3.53) results in

$$\mathbf{u}^T \bar{\mathbf{P}}_{xg} \frac{d\mathbf{u}}{dt} + a \left(\frac{1}{2} - \sigma_1 \right) \mathbf{u}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T \mathbf{u} + a \left(-\frac{1}{2} - \sigma_2 \right) \mathbf{u}^T \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T \mathbf{u} + a(\sigma_1 + \sigma_2) \mathbf{u}^T \mathbf{t}_{Lg} \mathbf{t}_{Rg}^T \mathbf{u} = 0. \quad (3.54)$$

Then, choosing $\sigma_1 = \frac{1}{2}$ and $\sigma_2 = -\frac{1}{2}$, we find that

$$\mathbf{u}^T \bar{\mathbf{P}}_{xg} \frac{d\mathbf{u}}{dt} = 0. \quad (3.55)$$

Next, we integrate in time to have

$$\|\mathbf{u}(T)\|_p^2 = \|\mathbf{u}(0)\|_p^2, \quad (3.56)$$

where $\|\mathbf{u}\|_p^2$ is the norm approximating L_2 norm. Therefore, the semi-discrete scheme (3.50) is stable.

3.3.2 Fourth-order Runge Kutta

In this section, we introduce the RK4 time marching method used throughout this thesis to integrate the ODEs that results from discretizing in space. To introduce the RK4 method, consider the following initial value problem.

$$\frac{d\mathcal{Y}}{dt} = \mathcal{F}(t, \mathcal{Y}), \quad \mathcal{Y}(t_0) = y_0. \quad (3.57)$$

Then, we choose a positive time step h , then we can approximate

$$\begin{aligned} y_{n+1} &= y_n + \frac{h}{6} (k_1 + 2k_2 + 2k_3 + k_4), \\ t_{n+1} &= t_n + h, \\ y_n &= \mathcal{Y}(t_n), \end{aligned} \tag{3.58}$$

where

$$\begin{aligned} k_1 &= \mathcal{F}(t_n, y_n), \\ k_2 &= \mathcal{F}\left(t_n + \frac{h}{2}, y_n + \frac{hk_1}{2}\right), \\ k_3 &= \mathcal{F}\left(t_n + \frac{h}{2}, y_n + \frac{hk_2}{2}\right), \\ k_4 &= \mathcal{F}(t_n + h, y_n + hk_3). \end{aligned} \tag{3.59}$$

3.3.3 Numerical Experiments for the Linear Advection Equation

In this subsection, we apply our discretization of the linear advection equation (2.6) and characterize its error properties. Specifically, we consider the following two linear advection problems with $a = 1$ [please check this]:

Problem 1:

$$\begin{aligned} \text{Domain: } &x \in [-\pi, \pi], \quad t > 0, \\ \text{Boundary condition: } &\mathcal{U}(-\pi, t) = \mathcal{U}(\pi, t), \\ \text{Initial condition: } &\mathcal{U}(x, 0) = \cos(3x), \end{aligned} \tag{3.60}$$

Problem 2:

$$\begin{aligned} \text{Domain: } &x \in [0, 1], \quad t > 0, \\ \text{Boundary condition: } &\mathcal{U}(0, t) = \cos(3t), \\ \text{Initial condition: } &\mathcal{U}(x, 0) = \cos(3x), \end{aligned} \tag{3.61}$$

where the exact solution for both problems is $\mathbf{u}_{ex} = \cos(-3x + 3t)$. We use CG-SBP operators to discretize the PDE through SBP-SAT technique based on the discretization in the section 3.3.1 and then use the fourth order Runge-Kutta scheme for time marching

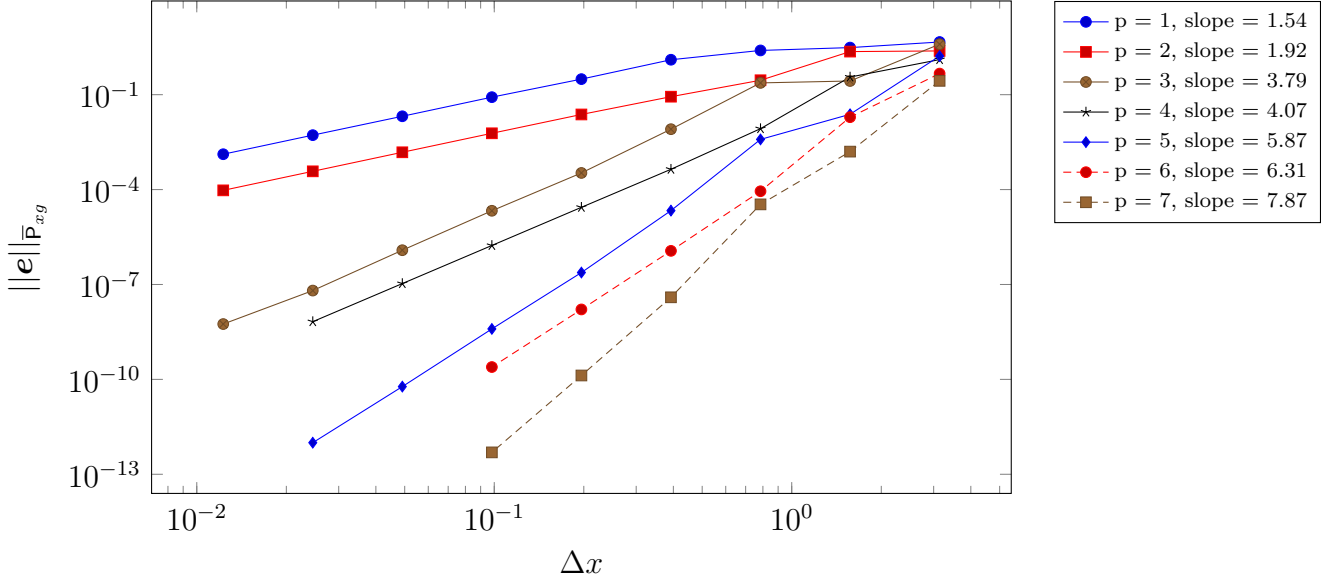


Figure 3.1: Convergence test of the linear advection equation discretized using the CG SBP-SAT method with periodic boundary conditions (Problem 1). The domain is discretized using multiple elements and Δx is computed by dividing the domain length in the x direction by the number of elements in the x direction. The coarsest mesh contains two elements while at each refinement level, the number of elements is doubled. The slopes are computed using the line of best fit through the last three data points.

from 0 to 1, with a time step of 10^{-5} . Note that for Problem 2 we only add a SAT to weakly enforce a boundary condition on the left of the domain as

$$\mathbf{SAT} = -\bar{\mathbf{P}}_{xg} \mathbf{t}_{Lg} (\mathbf{t}_{Lg}^T \mathbf{u}_g - \cos(3t)), \quad (3.62)$$

which can be proven to result in a stable semi-discrete form in exactly the same way as the periodic problem previously discussed. Then, we compute the error vector $\mathbf{e} = \mathbf{u}_{num} - \mathbf{u}_{ex}$ where $\mathbf{u}_{num}$ is the numerical solution and $\mathbf{u}_{ex}$ is the vector containing the exact solution at the mesh nodes. Finally, we compute the approximate L_2 error as follows:

$$\|\mathbf{e}\|_{\bar{\mathbf{P}}_{xg}} = (\mathbf{e}^T \bar{\mathbf{P}}_{xg} \mathbf{e})^{\frac{1}{2}}. \quad (3.63)$$

For Problem 1, we see from Figure 3.1, we see that the convergence rate is p for degree p operators when p is even and $\approx p + 1$ if p is odd with the exception of $p = 1$. Similarly, for Problem 2, we see from Figure 3.2, that the convergence rate is $\approx p + 1$ if the degree of the operator is odd, and p if the degree is even.

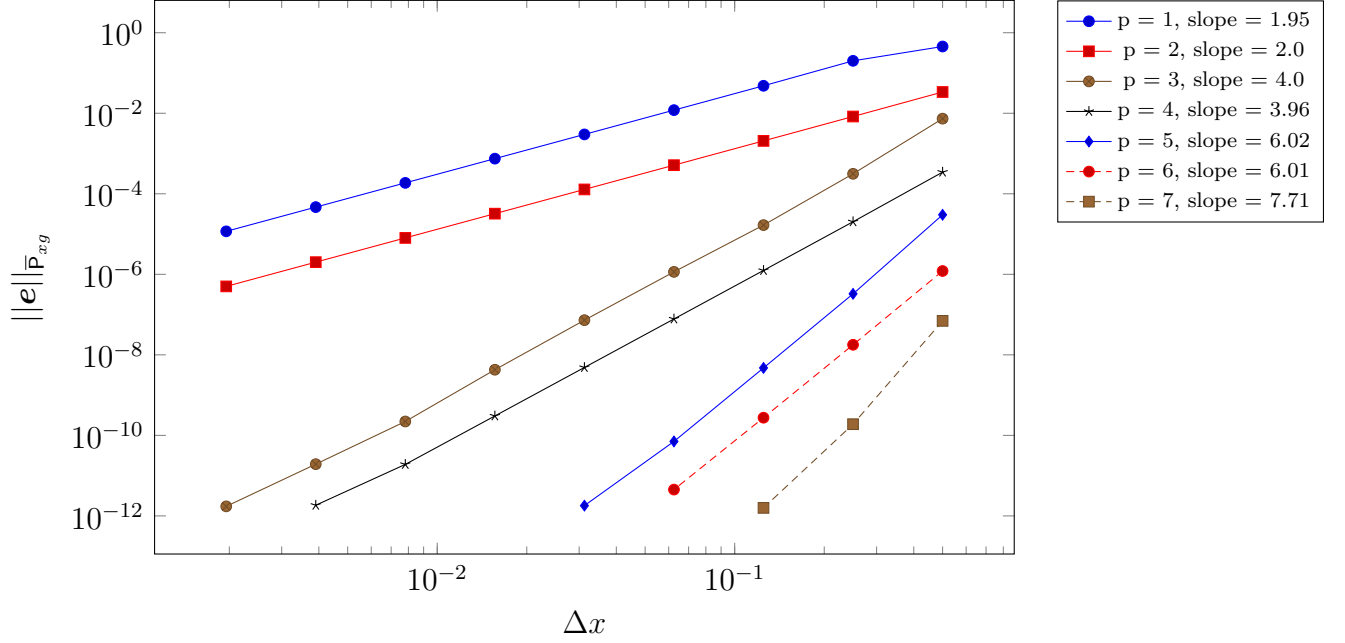


Figure 3.2: Convergence test of the linear advection equation using the CG SBP-SAT method with Dirichlet boundary condition (Problem 2). The domain is discretized using multiple elements and Δx is computed by dividing the domain length in the x direction by the number of elements in the x direction. The coarsest mesh contains two elements while at each refinement level, the number of elements is doubled. The slopes are computed using the line of best fit through the last three data points.

3.3.4 SBP-SAT Discretization of the Diffusion Equation

The SBP-SAT semi-discrete form of the diffusion equation with a homogenous Neumann boundary condition on the left and a homogenous Dirichlet boundary condition on the right is

$$\frac{d\mathbf{u}}{dt} - \bar{\mathbf{D}}_{2xg}\mathbf{u} = \sigma_1 \bar{\mathbf{P}}_{xg}^{-1} \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T \bar{\mathbf{D}}_{xg} \mathbf{u} + \sigma_2 \bar{\mathbf{P}}_{xg}^{-1} \bar{\mathbf{D}}_{xg}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T \mathbf{u}. \quad (3.64)$$

where the SATs are given as

$$\mathbf{SAT}_L := \sigma_1 \bar{\mathbf{P}}_{xg}^{-1} \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T \bar{\mathbf{D}}_{xg} \mathbf{u}, \quad \mathbf{SAT}_R := \sigma_2 \bar{\mathbf{P}}_{xg}^{-1} \bar{\mathbf{D}}_{xg}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T \mathbf{u}, \quad (3.65)$$

and σ_1 and σ_2 are the parameters for the SATs that will be chosen so that the scheme is stable. Here $\mathbf{SAT}_L$ imposes the left homogenous Neumann boundary condition and $\mathbf{SAT}_R$ imposes the right homogenous Dirichlet boundary condition weakly. To understand how the SATs encode the boundary conditions, note, for example, that $\mathbf{t}_{Lg}^T \bar{\mathbf{D}}_{xg} \mathbf{u} \approx \frac{\partial \mathcal{U}}{\partial x}(x_L) = 0$, and $\mathbf{t}_{Rg}^T \mathbf{u} \approx \mathcal{U}(x_R) = 0$. The LHS of (3.64) is the discretization of the linear diffusion equation using CG-SBP operators while the RHS of (3.64) are the SATs, which imposed the boundary conditions weakly. Again, the stability analysis of (3.64) follows identically from that at the continuous level. Thus, first we multiply (3.64) by $\mathbf{u}^T \bar{\mathbf{P}}_{xg}$ to obtain

$$\mathbf{u}^T \bar{\mathbf{P}}_{xg} \frac{d\mathbf{u}}{dt} - \mathbf{u}^T \bar{\mathbf{P}}_{xg} \bar{\mathbf{D}}_{2xg} \mathbf{u} = \sigma_1 \mathbf{u}^T \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T \bar{\mathbf{D}}_{xg} \mathbf{u} + \sigma_2 \mathbf{u}^T \bar{\mathbf{D}}_{xg}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T \mathbf{u}. \quad (3.66)$$

Next, we use the definition of $\bar{\mathbf{D}}_{2xg}$ given in 3.2.3 to obtain

$$\mathbf{u}^T \bar{\mathbf{P}}_{xg} \frac{d\mathbf{u}}{dt} - \mathbf{u}^T (-\bar{\mathbf{A}}_{xg} + \bar{\mathbf{E}}_{xg} \bar{\mathbf{D}}_{xg}) \mathbf{u} = \sigma_1 \mathbf{u}^T \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T \bar{\mathbf{D}}_{xg} \mathbf{u} + \sigma_2 \mathbf{u}^T \bar{\mathbf{D}}_{xg}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T \mathbf{u}. \quad (3.67)$$

Recall that $\bar{\mathbf{E}}_{xg} = \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T - \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T$, then, combining similar terms and rearranging (3.67) results in

$$\mathbf{u}^T \bar{\mathbf{P}}_{xg} \frac{d\mathbf{u}}{dt} = -\mathbf{u}^T \bar{\mathbf{A}}_{xg} \mathbf{u} + (\sigma_1 - 1) \mathbf{u}^T \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T \bar{\mathbf{D}}_{xg} \mathbf{u} + (1 + \sigma_2) \mathbf{u}^T \bar{\mathbf{D}}_{xg}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T \mathbf{u}. \quad (3.68)$$

Note that since $\bar{\mathbf{A}}_{xg}$ is a positive semi-definite matrix, then $-\mathbf{u}^T \bar{\mathbf{A}}_{xg} \mathbf{u}$ is a non-positive term, which can be dropped, then the (3.68) becomes

$$\mathbf{u}^T \bar{\mathbf{P}}_{xg} \frac{d\mathbf{u}}{dt} \leq (\sigma_1 - 1) \mathbf{u}^T \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T \bar{\mathbf{D}}_{xg} \mathbf{u} + (1 + \sigma_2) \mathbf{u}^T \bar{\mathbf{D}}_{xg}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T \mathbf{u}. \quad (3.69)$$

Then, we choose $\sigma_1 = 1, \sigma_2 = -1$ to obtain

$$\mathbf{u}^T \bar{\mathbf{P}}_{xg} \frac{d\mathbf{u}}{dt} \leq 0. \quad (3.70)$$

Applying chain rule, (3.70) can be rewritten as

$$\frac{1}{2} \frac{d}{dt} \mathbf{u}^T \bar{\mathbf{P}}_{xg} \mathbf{u} \leq 0. \quad (3.71)$$

Finally, integrating with respect to time results in

$$\|\mathbf{u}(T)\|^2 \leq \|\mathbf{u}(0)\|^2. \quad (3.72)$$

Thus, the scheme is stable. Note that we can use either form of $\bar{\mathbf{A}}_{xg}$ and arrive at the same result. A similar analysis of the SBP-SAT discretization of the diffusion equation with Dirchlet boundary conditions weakly imposed on both ends demonstrates that the resultant semi-discrete form is stable. In the next subsection, numerical experiments are performed to demonstrate the convergence rates of the proposed schemes.

3.3.5 Numerical Experiments for the Diffusion Equation

To study the convergence properties of the schemes for the diffusion equation (2.13), we consider the following two problems.

Problem 1:

$$\begin{aligned} \text{Domain: } x &\in \left[0, \frac{3\pi}{2}\right], \quad t > 0, \\ \text{Boundary conditions: } \frac{\partial \mathcal{U}}{\partial x}(0, t) &= 0, \quad \mathcal{U}\left(\frac{3\pi}{2}, t\right) = 0, \\ \text{Initial condition: } \mathcal{U}(x, 0) &= \cos(x), \end{aligned} \quad (3.73)$$

Problem 2:

$$\begin{aligned} \text{Domain: } x &\in \left[0, \frac{3\pi}{2}\right], \quad t > 0, \\ \text{Boundary conditions: } \mathcal{U}(0, t) &= 0, \quad \mathcal{U}\left(\frac{3\pi}{2}, t\right) = 0, \\ \text{Initial condition: } \mathcal{U}(x, 0) &= \cos(x), \end{aligned} \quad (3.74)$$

where the exact solution is $\mathbf{u}_{\text{ex}} = \cos(x)e^{-t}$ for both problems. In the numerical tests, we will consider the two options for constructing the second derivative as well as various

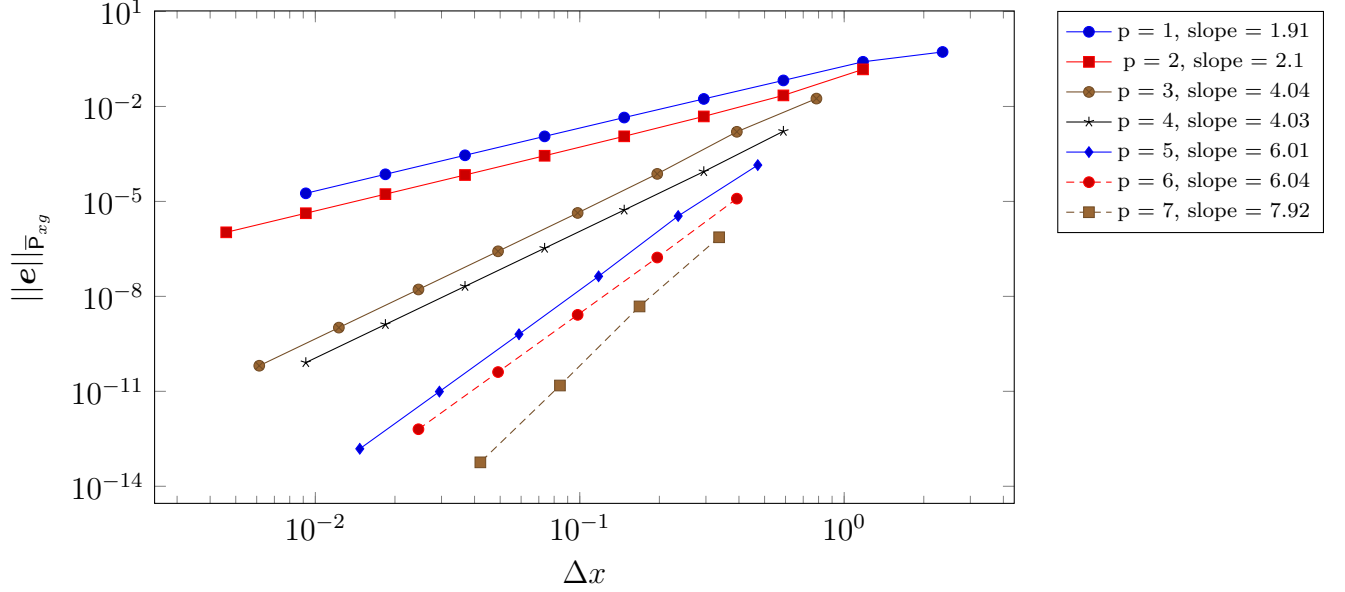


Figure 3.3: Convergence test of the diffusion equation discretized using the CG SBP-SAT method and $\bar{A}_{xg} = \bar{D}_{xg}^T \bar{P}_{xg} \bar{D}_{xg}$ with a homogenous Neumann boundary condition and a homogenous Dirichlet boundary condition on the left and right boundaries, respectively (Problem 1). The domain is discretized using multiple elements and Δx is computed by dividing the domain length in the x direction by the number of elements in the x direction. The coarsest mesh contains two elements while at each refinement level, the number of elements is doubled. The slopes are computed using the line of best fit through the last three data points.

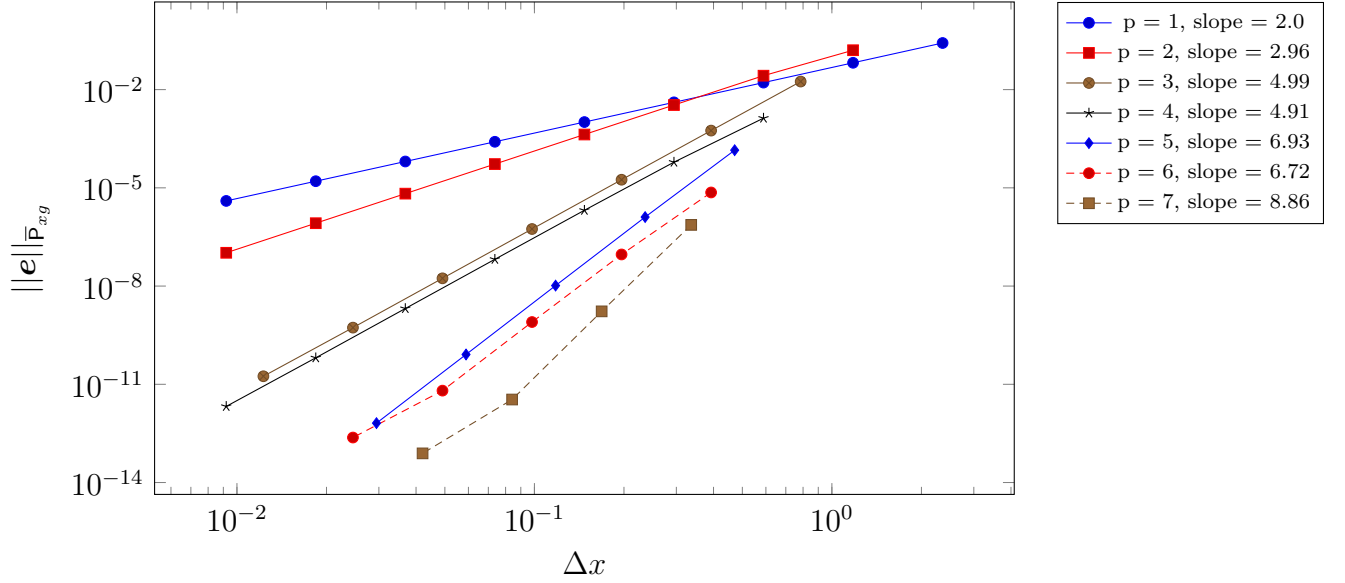


Figure 3.4: Convergence test of the diffusion equation discretized using the CG SBP-SAT method and $\bar{\mathbf{A}}_{xg} = \sum_{i=1}^N \mathbf{R}_i^T \bar{\mathbf{D}}_x^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \mathbf{R}_i$ with a homogenous Neumann boundary condition and a homogenous Dirichlet boundary condition on the left and right boundaries, respectively (Problem 1). The domain is discretized using multiple elements and Δx is computed by dividing the domain length in the x direction by the number of elements in the x direction. The coarsest mesh contains two elements while at each refinement level, the number of elements is doubled. The slopes are computed using the line of best fit through the last three data points.

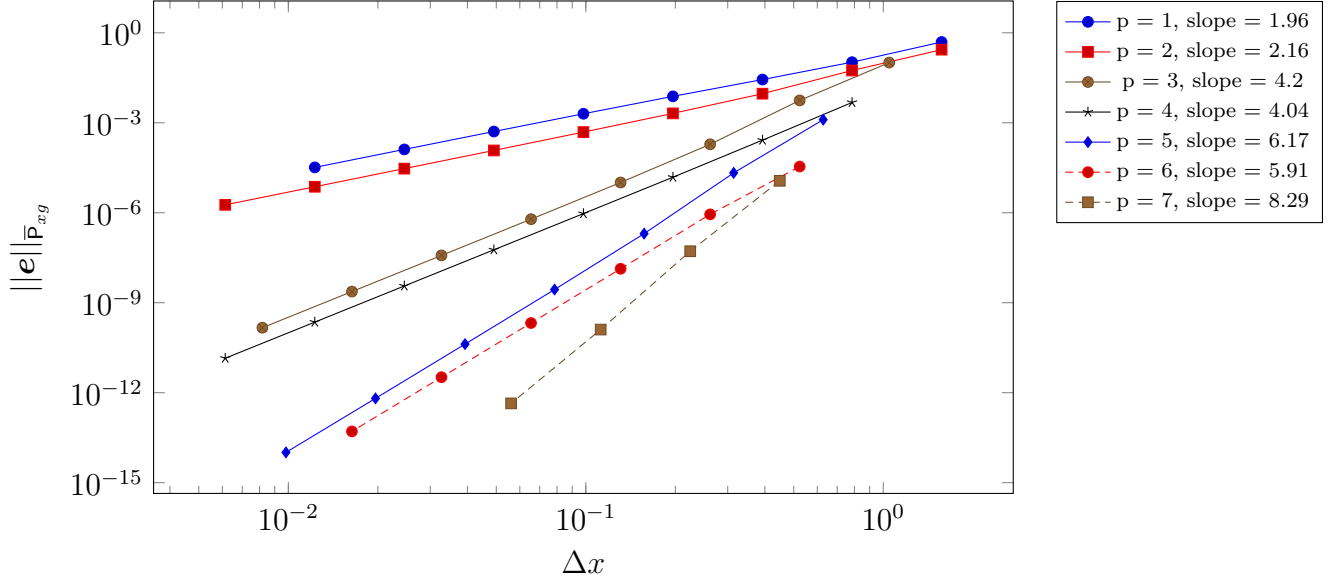


Figure 3.5: Convergence test of the diffusion equation discretized using the CG SBP-SAT method and $\bar{A}_{xg} = \bar{D}_{xg}^T \bar{P}_{xg} \bar{D}_{xg}$ with homogenous Dirichlet boundary condition on both ends (Problem 2). The domain is discretized using multiple elements and Δx is computed by dividing the domain length in the x direction by the number of elements in the x direction. The coarsest mesh contains two elements while at each refinement level, the number of elements is doubled. The slopes are computed using the line of best fit through the last three data points.

degree SBP operators. The setup of the convergence study is identical to that performed for the linear advection equation.

For problem (3.74), Figure 3.3 demonstrates that the convergence rate obtained using $\bar{A}_{xg} = \bar{D}_{xg}^T \bar{P}_{xg} \bar{D}_{xg}$ is $p + 1$ if p is odd, with the exception of $p = 1$, and p if p is even. From the Figure 3.4, we find the convergence rate obtained for $\bar{A}_{xg} = \sum_{i=1}^N R_i^T \bar{D}_x^T \bar{P}_x \bar{D}_x R_i$ is $p + 2$ if p is odd and $p + 1$ if p is even.

The results of the numerical experiments for the problem (3.74) are shown in the Figures 3.5 and 3.6. From the Figure 3.5, the convergence rate resulting from using $\bar{A}_{xg} = \bar{D}_{xg}^T \bar{P}_{xg} \bar{D}_{xg}$ is $p + 1$ if p is odd and p if p is even. From the Figure 3.6, the convergence rate resulting from using $\bar{A}_{xg} = \sum_{i=1}^N R_i^T \bar{D}_x^T \bar{P}_x \bar{D}_x R_i$ is $p + 2$ if p is odd, with the exception of $p = 1$, and $p + 1$ if p is even.

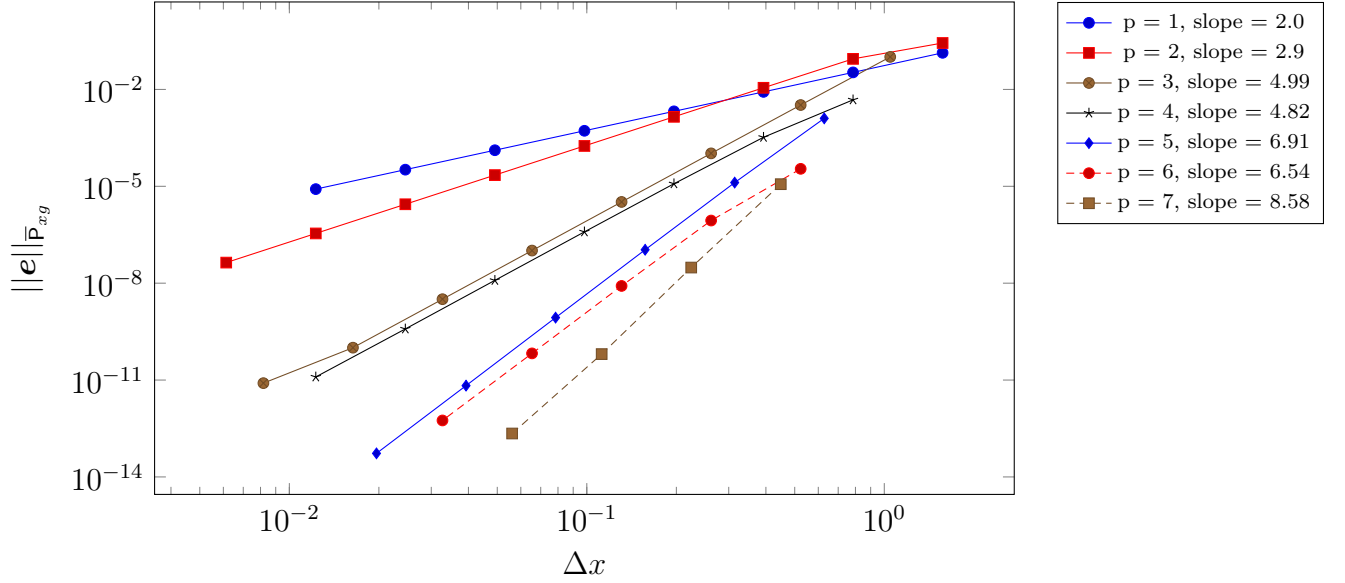


Figure 3.6: Convergence test of the diffusion equation discretized using CG SBP-SAT method and $\bar{A}_{xg} = \sum_{i=1}^N \mathbf{R}_i^T \bar{\mathbf{D}}_x^T \bar{\mathbf{P}}_x \bar{\mathbf{D}}_x \mathbf{R}_i$ with homogenous Dirichlet boundary condition on both ends (Problem 2). The domain is discretized using multiple elements and Δx is computed by dividing the domain length in the x direction by the number of elements in the x direction. The coarsest mesh contains two elements while at each refinement level, the number of elements is doubled. The slopes are computed using the line of best fit through the last three data points. The slopes are computed using the line of best fit through the last three data points.

Based on the Figures 3.3, 3.4, 3.5 and 3.6, we find that $\bar{A}_{xg} = \sum_{i=1}^N R_i^T \bar{D}_x^T \bar{P}_x \bar{D}_x R_i$ performs better on the convergence rate. Therefore, we will use $\bar{A}_{xg} = \sum_{i=1}^N R_i^T \bar{D}_x^T \bar{P}_x \bar{D}_x R_i$ to discretize the KZK equation.

3.3.6 SBP SAT Discretization of the Burgers' equation

The Burgers' equation with homogenous Dirichlet boundary conditions on both ends can be discretized as follows:

$$\frac{d\mathbf{u}}{dt} + \frac{1}{3}\bar{D}_{xg}[\mathbf{u}]\mathbf{u} + \frac{1}{3}[\mathbf{u}]\bar{D}_{xg}\mathbf{u} = \sigma_1 \bar{P}_{xg}^{-1} \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T [\mathbf{u}]\mathbf{u} + \sigma_2 \bar{P}_{xg}^{-1} \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T [\mathbf{u}]\mathbf{u}, \quad (3.75)$$

where $[\mathbf{u}] := \text{diag}(u_1, \dots, u_l)$, and the SATs are given as

$$\mathbf{SAT}_L := \sigma_1 \bar{P}_{xg}^{-1} \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T [\mathbf{u}]\mathbf{u}, \quad \mathbf{SAT}_R := \sigma_2 \bar{P}_{xg}^{-1} \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T [\mathbf{u}]\mathbf{u}, \quad (3.76)$$

and σ_1 and σ_2 are the parameters for the SATs that will be chosen so that the scheme is stable. Here $\mathbf{SAT}_L$ and $\mathbf{SAT}_R$ imposes the homogenous Dirichlet boundary conditions on the left and right boundaries, respectively. The LHS of (3.75) is the discretization of the Burgers' equation using CG-SBP operators while the RHS of (3.75) are the SATs, which imposed the homogenous dirchlet boundary conditions weakly. Then, to prove stability, we multiply (3.75) by $\mathbf{u}^T \bar{P}_{xg}$ to obtain

$$\mathbf{u}^T \bar{P}_{xg} \frac{d\mathbf{u}}{dt} + \frac{1}{3} \mathbf{u}^T \bar{Q}_{xg} [\mathbf{u}]\mathbf{u} + \frac{1}{3} \mathbf{u}^T \bar{P}_{xg} [\mathbf{u}] \bar{D}_{xg} \mathbf{u} = \sigma_1 \mathbf{u}^T \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T [\mathbf{u}]\mathbf{u} + \sigma_2 \mathbf{u}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T [\mathbf{u}]\mathbf{u}. \quad (3.77)$$

Recollecting that $[\mathbf{u}]$ and $\bar{P}_{xg}$ are diagonal matrices and the transpose of a scalar is itself, then (3.77) can be rewritten as

$$\mathbf{u}^T \bar{P}_{xg} \frac{d\mathbf{u}}{dt} + \frac{1}{3} \mathbf{u}^T \bar{Q}_{xg} [\mathbf{u}]\mathbf{u} + \frac{1}{3} \mathbf{u}^T \bar{Q}_{xg}^T [\mathbf{u}]\mathbf{u} = \sigma_1 \mathbf{u}^T \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T [\mathbf{u}]\mathbf{u} + \sigma_2 \mathbf{u}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T [\mathbf{u}]\mathbf{u}. \quad (3.78)$$

Then, rearranging terms and using the SBP property $\bar{Q}_{xg} + \bar{Q}_{xg}^T = \bar{E}_{xg} = \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T - \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T$ (3.78) can be simplified as

$$\mathbf{u}^T \bar{P}_{xg} \frac{d\mathbf{u}}{dt} = \left(\sigma_1 + \frac{1}{3} \right) \mathbf{u}^T \mathbf{t}_{Lg} \mathbf{t}_{Lg}^T [\mathbf{u}]\mathbf{u} + \left(\sigma_2 - \frac{1}{3} \right) \mathbf{u}^T \mathbf{t}_{Rg} \mathbf{t}_{Rg}^T [\mathbf{u}]\mathbf{u}. \quad (3.79)$$

Choosing the parameters $\sigma_1 = -\frac{1}{3}$, and $\sigma_2 = \frac{1}{3}$ to simplify (3.79) as

$$\mathbf{u}^T \bar{P}_{xg} \frac{d\mathbf{u}}{dt} = 0. \quad (3.80)$$

Integrating in time, we have that

$$\|\mathbf{u}(T)\|^2 = \|\mathbf{u}(0)\|^2. \quad (3.81)$$

Therefore, the scheme (3.75) for the Burgers' equation with homogenous Dirichlet boundary conditions is stable. In the next subsection, numerical experiments are performed to demonstrate the convergence rates of the proposed schemes.

3.3.7 Numerical Experiments of the Burgers' Equation

To determine the convergence rate of our scheme for the Burgers' equation, we use a manufacture solution. Consider the following problem for the Burgers equation, where the manufacture solution $\mathcal{U}_{MMS} = \sin(x)e^{-t}$.

$$\begin{aligned} \frac{\partial \mathcal{U}}{\partial t} + \mathcal{U} \frac{\partial \mathcal{U}}{\partial x} &= -\sin(x)e^{-t} + \sin(x)\cos(x)e^{-2t}, \quad x \in [0, \pi], \quad t > 0, \\ \mathcal{U}(0, t) &= 0, \quad \mathcal{U}(\pi, t) = 0, \\ \mathcal{U}(x, 0) &= \sin(x). \end{aligned} \quad (3.82)$$

The setup for the convergence study is the same as with previous test with the error vector now is defined as $\mathbf{e} = \mathbf{u}_{num} - \mathbf{u}_{MMS}$. The convergence rates are given in Figure 3.7 and we find that they are $p + \frac{1}{2}$ if p is odd and p if p is even.

3.4 Chapter Summary

In this chapter, we introduced the definition of SBP operators and explained how to construct CG operators that satisfy this definition. Moreover, we preformed a continuous and discrete stability analysis of linear advection, linear diffusion, and Burgers' equation. The discretizations presented in this chapter provide the basic building blocks for constructing the discretization of the KZK equations that will be considered in the next chapter.

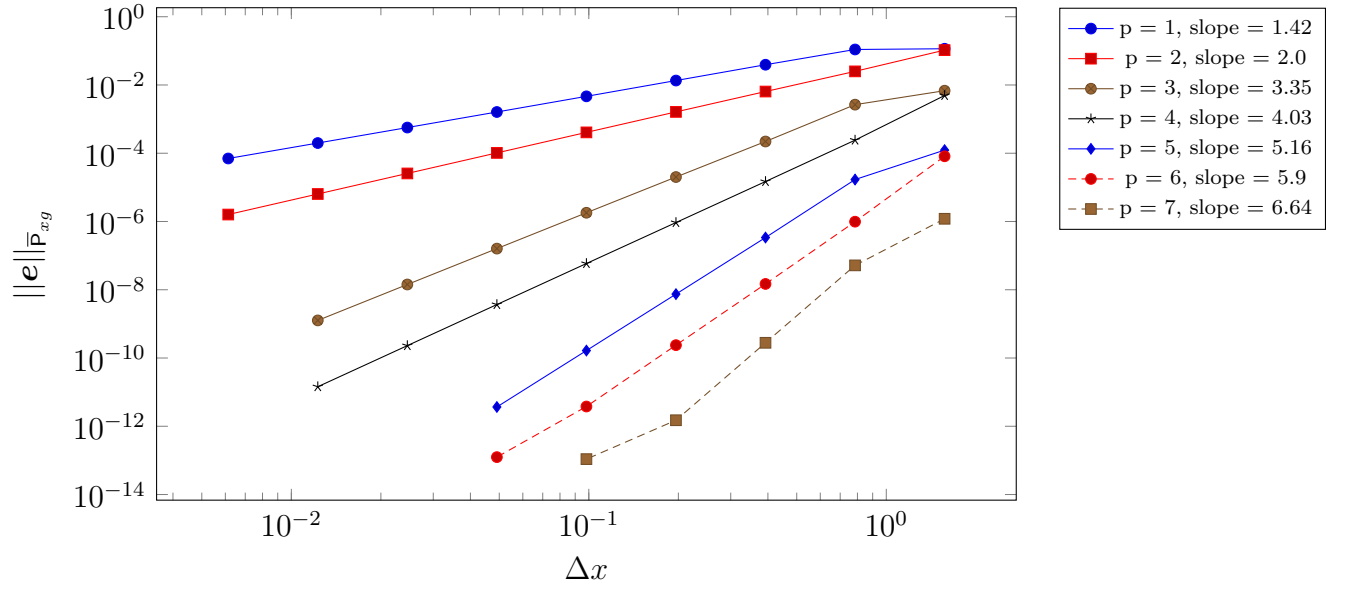


Figure 3.7: Convergence test of Burgers' equation discretized using CG SBP-SAT method with homogenous Dirichlet boundary condition on both ends. The domain is discretized using multiple elements and Δx is computed by dividing the domain length in the x direction by the number of elements in the x direction. The coarsest mesh contains two elements while at each refinement level, the number of elements is doubled. The slopes are computed using the line of best fit through the last three data points.

Chapter 4

CG-SBP-SAT Discretization of the KZK Equation

This chapter discusses our discretization approach for the KZK equation. As in previous chapters, the starting point is to examine the continuous stability of the KZK equation. We use this to motivate the construction of our scheme such that we can mimic this continuous stability analysis at the semi-discrete level. Of importance to doing so, and a major contribution of this thesis, is developing special second derivative operators. In order to discretize the KZK equation, we demonstrate how to extend the global one dimensional CG-SBP operators into multiple dimensions using tensor products. Finally, boundary conditions are imposed using SATs, motivated from our discretization of the linear advection equation, linear diffusion equation, and Burgers' equation.

4.1 Continuous Stability Analysis of the KZK Equation

The three-dimensional KZK equation for pressure $\mathcal{U}$ has the following form [4]:

$$\frac{\partial^2 \mathcal{U}}{\partial t' \partial z} - \frac{\beta}{2\rho c_0^3} \frac{\partial^2 \mathcal{U}^2}{\partial t'^2} - \frac{\delta}{2c_0^3} \frac{\partial^3 \mathcal{U}}{\partial t'^3} - \frac{c_0}{2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \mathcal{U} = 0. \quad (4.1)$$

In this thesis, we assume $\mathcal{U}$ has compact support on the domain. Here $t' = t - z/c_0$ is the retarded time, where t is the time and c_0 is the sound speed. The Cartesian coordinates are x , y , and z , where the z coordinate represents the direction of wave propagation, see

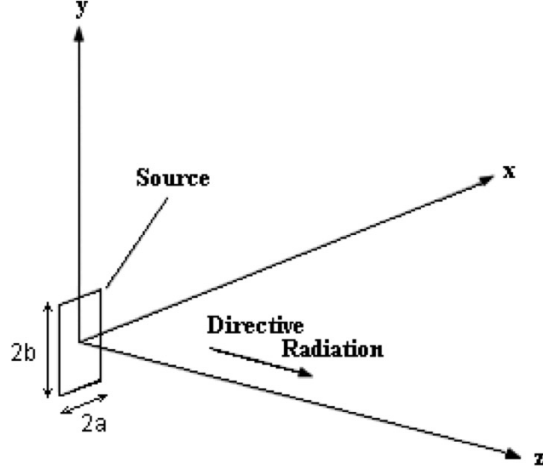


Figure 4.1: Geometry and systems of coordinates [45].

Figure 4.1. The coefficient of nonlinearity is defined as $\beta = 1 + \frac{B}{A}$, where $\frac{B}{A}$ is the nonlinear parameter of the medium. Furthermore, $\delta = \frac{1}{\rho} \left(\frac{4\mu}{3} + \mu_\beta + k \left(\frac{1}{c_v} - \frac{1}{c_p} \right) \right)$ is the diffusivity of the sound where ρ is the ambient density, k is the thermal conductivity, μ , μ_β , c_v and c_p are shear viscosity, bulk viscosity, the specific heat at constant volume, and the specific heat at constant pressure, respectively. Applying the operator $\partial_{t'}^{-1}$ to (4.1), and using the compact support of $\mathcal{U}$ on the domain, leads to

$$\frac{\partial \mathcal{U}}{\partial z} - \frac{\beta}{2\rho c_0^3} \frac{\partial \mathcal{U}^2}{\partial t'} - \frac{\delta}{2c_0^3} \frac{\partial^2 \mathcal{U}}{\partial t'^2} - \frac{c_0}{2} \partial_{t'}^{-1} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \mathcal{U} = 0. \quad (4.2)$$

We non-dimensionalize (4.2) using the following dimensionless variables [95, 55]:

$$\begin{aligned} \sigma &= z/d, \\ X &= x/a, \\ Y &= y/b, \\ \tau &= \omega_0 t', \\ \mathcal{P} &= \mathcal{U}/p_0, \end{aligned} \quad (4.3)$$

where d is the focal length in the direction of propagation, the quantities a and b are the size of the source aperture in the x and y direction, respectively. The working frequency of the source pulse is ω_0 and peak source pressure is p_0 . Then, substituting the variables

(4.3) into (4.2) results in [95, 17]

$$\frac{\partial \mathcal{P}}{\partial \sigma} - \tilde{N} \mathcal{P} \frac{\partial \mathcal{P}}{\partial \tau} - A \frac{\partial^2 \mathcal{P}}{\partial \tau^2} - \frac{1}{4} \partial_\tau^{-1} \left(\frac{1}{G_x} \frac{\partial^2}{\partial X^2} + \frac{1}{G_y} \frac{\partial^2}{\partial Y^2} \right) \mathcal{P} = 0. \quad (4.4)$$

In this thesis, we will exclusively consider hyperrectangles for the spatial domain, i.e., $\Omega := (X, Y, \tau) \in [X_{min}, X_{max}] \times [Y_{min}, Y_{max}] \times [\tau_{min}, \tau_{max}]$, where σ is taken as an artificial temporal variable. Moreover, $G_x = \frac{k_0 a^2}{2d}$, $G_y = \frac{k_0 b^2}{2d}$, $\tilde{N} = \frac{d}{\bar{z}}$, and $A = \alpha_0 d$ are dimensionless coefficients, where $k_0 = \frac{\omega_0}{c_0}$ is the wave number, the wave shock formation distance is defined as $\bar{z} = \frac{\rho_0 c_0^3}{\beta \omega_0 p_0}$ and $\alpha_0 = \frac{\delta \omega_0^2}{2c_0^3}$ is the thermoviscous absorption coefficient at the working frequency.

4.1.1 Source and Boundary Conditions

The source condition of KZK equation is constructed by setting the time waveforms at $\sigma = 0$. In this thesis, we consider the following source condition, which is a parabolic approximation of the ultrasound beam [55, 95]:

$$\mathcal{U}(x, y, t) = p_0 \mathcal{F} \left(t + \frac{x^2}{2c_0 d_X} + \frac{y^2}{2c_0 d_Y} \right) \mathcal{G}(x, y), \quad z = 0. \quad (4.5)$$

In dimensionless variables, the source condition can be written as follows:

$$\mathcal{P}(X, Y, \tau) = \mathcal{F}(\tau + G_{XS} X^2 + G_{YS} Y^2) \mathcal{G}(X, Y), \quad \sigma = 0, \quad (4.6)$$

where $G_{XS} = \frac{G_x d}{d_X}$ and $G_{YS} = \frac{G_y d}{d_Y}$ and $\mathcal{G}(x, y)$ is the shading function [55, 95, 17, 45]. Here we use

$$\mathcal{G}(X, Y) = \begin{cases} 1 & \text{if } |X| \leq 1 \text{ and } |Y| \leq 1, \\ 0 & \text{otherwise.} \end{cases} \quad (4.7)$$

Next, we need to choose appropriate boundary conditions, where based on experiments performed on focused ultrasound [95, 45, 17, 55] two natural candidates for boundary conditions emerge.

Case 1. Assume we have a large enough box, which contains all the ultrasound wave. This gives us zero pressure at the faces of the domain and thus, the following boundary conditions:

$$\begin{aligned} \mathcal{P}(X_{max}, Y, \tau, \sigma) &= 0, & \mathcal{P}(X_{min}, Y, \tau, \sigma) &= 0, \\ \mathcal{P}(X, Y_{max}, \tau, \sigma) &= 0, & \mathcal{P}(X, Y_{min}, \tau, \sigma) &= 0, \\ \mathcal{P}(X, Y, \tau_{max}, \sigma) &= 0, & \mathcal{P}(X, Y, \tau_{min}, \sigma) &= 0. \end{aligned} \quad (4.8)$$

Case 2. Assume the problem is axisymmetric, therefore, we can consider a smaller equivalent problem constructed by halving the original domain along each axis of symmetry. Then, we set homogeneous Neumann boundary conditions for the faces belonging to planes of symmetry of the new domain. For the remaining boundary faces, we use homogeneous Dirichlet boundary conditions, thus, the full set of boundary conditions is

$$\begin{aligned} \mathcal{P}(X_{max}, Y, \tau, \sigma) &= 0, & \frac{\partial \mathcal{P}}{\partial X}(X_{min}, Y, \tau, \sigma) &= 0, \\ \mathcal{P}(X, Y_{max}, \tau, \sigma) &= 0, & \frac{\partial \mathcal{P}}{\partial Y}(X, Y_{min}, \tau, \sigma) &= 0, \\ \mathcal{P}(X, Y, \tau_{max}, \sigma) &= 0, & \mathcal{P}(X, Y, \tau_{min}, \sigma) &= 0 \end{aligned} \quad (4.9)$$

Next, we prove that the non-dimensional form of the KZK equation (4.4) with the either boundary conditions (4.8) or (4.9) is stable.

Theorem 4.1.1. *The solution to the KZK equation (4.2) along with boundary conditions (4.9) or (4.8) and source condition $\mathcal{P}_0 := \mathcal{P}(X, Y, \tau, \sigma_{min})$ satisfies:*

$$||\mathcal{P}(\sigma_{max})||^2 \leq ||\mathcal{P}_0||^2,$$

and thus, the KZK equation with either of these boundary conditions is stable.

Proof. First, we multiply (4.4) by $\mathcal{P}$, integrate over Ω , and then use Leibniz' rule on the last term to obtain

$$\int_{\Omega} \mathcal{P} \frac{\partial \mathcal{P}}{\partial \sigma} d\Omega = A \int_{\Omega} \mathcal{P} \frac{\partial \mathcal{P}^2}{\partial \tau} d\Omega + \tilde{N} \int_{\Omega} \mathcal{P} \frac{\partial^2 \mathcal{P}}{\partial \tau^2} d\Omega + \frac{1}{4} \int_{\Omega} \mathcal{P} \left(\frac{1}{G_x} \frac{\partial^2}{\partial X^2} + \frac{1}{G_y} \frac{\partial^2}{\partial Y^2} \right) \partial_{\tau}^{-1} \mathcal{P} d\Omega. \quad (4.10)$$

Next, we apply integration by parts and Leibniz' rule to obtain

$$\begin{aligned} \int_{\Omega} \mathcal{P} \frac{\partial \mathcal{P}}{\partial \sigma} d\Omega &= \frac{A}{3} \int_{X_{min}}^{X_{max}} \int_{Y_{min}}^{Y_{max}} \mathcal{P}^3 \Big|_{\tau_{min}}^{\tau_{max}} dY dX \\ &+ \tilde{N} \int_{X_{min}}^{X_{max}} \int_{Y_{min}}^{Y_{max}} \mathcal{P} \frac{\partial \mathcal{P}}{\partial \tau} \Big|_{\tau_{min}}^{\tau_{max}} dY dX - \tilde{N} \int_{\Omega} \left(\frac{\partial \mathcal{P}}{\partial \tau} \right)^2 d\Omega \\ &+ \frac{1}{G_y} \int_{X_{min}}^{X_{max}} \int_{\tau_{min}}^{\tau_{max}} \mathcal{P} \partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial Y} \Big|_{Y_{min}}^{Y_{max}} d\tau dX - \frac{1}{G_y} \int_{\Omega} \frac{\partial \mathcal{P}}{\partial Y} \partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial Y} d\Omega \\ &+ \frac{1}{G_x} \int_{Y_{min}}^{Y_{max}} \int_{\tau_{min}}^{\tau_{max}} \mathcal{P} \partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial X} \Big|_{X_{min}}^{X_{max}} d\tau dY - \frac{1}{G_x} \int_{\Omega} \frac{\partial \mathcal{P}}{\partial X} \partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial X} d\Omega. \end{aligned} \quad (4.11)$$

Then, applying the boundary conditions (4.9) to (4.11) results in

$$\int_{\Omega} \mathcal{P} \frac{\partial \mathcal{P}}{\partial \sigma} d\Omega = -\tilde{N} \int_{\Omega} \left(\frac{\partial \mathcal{P}}{\partial \tau} \right)^2 d\Omega - \frac{1}{G_y} \int_{\Omega} \frac{\partial \mathcal{P}}{\partial Y} \partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial Y} d\Omega - \frac{1}{G_x} \int_{\Omega} \frac{\partial \mathcal{P}}{\partial X} \partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial X} d\Omega. \quad (4.12)$$

Dropping the negative semi-definite terms results in

$$\int_{\Omega} \mathcal{P} \frac{\partial \mathcal{P}}{\partial \sigma} d\Omega \leq -\frac{1}{G_y} \int_{\Omega} \frac{\partial \mathcal{P}}{\partial Y} \partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial Y} d\Omega - \frac{1}{G_x} \int_{\Omega} \frac{\partial \mathcal{P}}{\partial X} \partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial X} d\Omega. \quad (4.13)$$

To proceed, recall the definition of the inverse operator (3.20), via the fundamental theorem of calculus we have the following identity:

$$\frac{\partial}{\partial t'} (\partial_{t'}^{-1} f) = f. \quad (4.14)$$

Then, using this identity on the RHS of (4.13), results in

$$\int_{\Omega} \mathcal{P} \frac{\partial \mathcal{P}}{\partial \sigma} d\Omega \leq -\frac{1}{G_y} \int_{\Omega} \frac{\partial}{\partial \tau} \left(\partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial Y} \right) \left(\partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial Y} \right) d\Omega - \frac{1}{G_x} \int_{\Omega} \frac{\partial}{\partial \tau} \left(\partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial X} \right) \left(\partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial X} \right) d\Omega. \quad (4.15)$$

Next, applying integration by parts to (4.15) results in

$$\begin{aligned} \frac{1}{2} \frac{\partial}{\partial \sigma} \int_{\Omega} \mathcal{P}^2 d\Omega &\leq -\frac{1}{2G_y} \int_{X_{min}}^{X_{max}} \int_{Y_{min}}^{Y_{max}} \left(\partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial Y} \right)^2 \Big|_{\tau_{min}}^{\tau_{max}} dX dY \\ &\quad - \frac{1}{2G_x} \int_{X_{min}}^{X_{max}} \int_{Y_{min}}^{Y_{max}} \left(\partial_{\tau}^{-1} \frac{\partial \mathcal{P}}{\partial X} \right)^2 \Big|_{\tau_{min}}^{\tau_{max}} dX dY. \end{aligned} \quad (4.16)$$

Using the definition of ∂_{τ}^{-1} , we can expand (4.16) as follows:

$$\begin{aligned} \frac{1}{2} \frac{d}{d\sigma} \int_{\Omega} \mathcal{P}^2 d\Omega &\leq -\frac{1}{2G_y} \int_{X_{min}}^{X_{max}} \int_{Y_{min}}^{Y_{max}} \left(\int_{\tau_{min}}^{\tau_{max}} \frac{\partial \mathcal{P}}{\partial Y} d\tau \right)^2 dX dY \\ &\quad + \frac{1}{2G_y} \int_{X_{min}}^{X_{max}} \int_{Y_{min}}^{Y_{max}} \left(\int_{\tau_{min}}^{\tau_{max}} \frac{\partial \mathcal{P}}{\partial Y} d\tau \right)^2 dX dY \\ &\quad - \frac{1}{2G_x} \int_{X_{min}}^{X_{max}} \int_{Y_{min}}^{Y_{max}} \left(\int_{\tau_{min}}^{\tau_{max}} \frac{\partial \mathcal{P}}{\partial X} d\tau \right)^2 dX dY \\ &\quad + \frac{1}{2G_x} \int_{X_{min}}^{X_{max}} \int_{Y_{min}}^{Y_{max}} \left(\int_{\tau_{min}}^{\tau_{max}} \frac{\partial \mathcal{P}}{\partial X} d\tau \right)^2 dX dY. \end{aligned} \quad (4.17)$$

Then we can simplify (4.17) and obtain

$$\frac{d}{d\sigma} \int_{\Omega} \mathcal{P}^2 d\Omega \leq 0. \quad (4.18)$$

Integrating (4.18) over σ and applying the source condition results in

$$||\mathcal{P}(\sigma_{max})||^2 \leq ||\mathcal{P}_0||^2. \quad (4.19)$$

Hence, the KZK equation with the boundary conditions (4.9) and source condition (4.6) is stable. The analysis for boundary conditions (4.8) follow similarly. $\square$

In the next section, we construct appropriate SBP operators and SATs that result in a semi-discrete form that enables a stability proof that matches the continuous stability proof presented above in a one-to-one fashion. In this thesis, we will only consider the second set of boundary conditions (4.9) for the discretization as they require less computational cost.

4.2 CG-SBP-SAT Discretization of the KZK Equation

Thus far, we have constructed element-wise SBP operators that are extended to global CG-SBP operators over a one-dimensional mesh constructed from elements. In this section, we extend these ideas to Cartesian meshes constructed from tensor-product elements. For this purpose, we introduce the definition of a tensor product.

Definition 4.2.1. *The tensor product of two matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $\mathbf{B} \in \mathbb{R}^{p \times q}$ is*

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \cdots & \cdots & a_{1m}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \cdots & \cdots & a_{2m}\mathbf{B} \\ \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ a_{n1}\mathbf{B} & a_{n2}\mathbf{B} & \cdots & \cdots & a_{nm}\mathbf{B} \end{bmatrix} \in \mathbb{R}^{mp \times nq}.$$

Here, we list some key properties of tensor products. Consider matrices $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}, \mathbf{E}$, and $\mathbf{F}$, we have that

$$(\mathbf{A} \otimes \mathbf{B})^{-1} = \mathbf{A}^{-1} \otimes \mathbf{B}^{-1}, \quad (4.20a)$$

$$(A \otimes B)^T = A^T \otimes B^T, \quad (4.20b)$$

$$(A \otimes B \otimes C) + (A \otimes B \otimes D) = A \otimes B \otimes (C + D), \quad (4.20c)$$

$$(A \otimes B \otimes C)(D \otimes E \otimes F) = AD \otimes BE \otimes CF, \quad (4.20d)$$

where the last two properties hold for matrices of appropriate size.

Using tensor product we construct three-dimensional SBP operators for hyperrectangles (i.e., $\Omega = [X_{min}, X_{max}] \times [Y_{min}, Y_{max}] \times [\tau_{min}, \tau_{max}]$) that are constructed from our one-dimensional CG-SBP operators as follows:

$$\begin{aligned} D_X &:= \bar{D}_{Xg} \otimes \bar{I}_{Yg} \otimes \bar{I}_{\tau g}, & D_Y &:= \bar{I}_{Xg} \otimes \bar{D}_{Yg} \otimes \bar{I}_{\tau g}, & D_\tau &:= \bar{I}_{Xg} \otimes \bar{I}_{Yg} \otimes \bar{D}_{\tau g}, \\ A_X &:= \bar{A}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{P}_{\tau g}, & A_Y &:= \bar{P}_{Xg} \otimes \bar{A}_{Yg} \otimes \bar{P}_{\tau g}, & A_\tau &:= \bar{P}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{A}_{\tau g}, \\ Q_X &:= \bar{Q}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{P}_{\tau g}, & Q_Y &:= \bar{P}_{Xg} \otimes \bar{Q}_{Yg} \otimes \bar{P}_{\tau g}, & Q_\tau &:= \bar{P}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{Q}_{\tau g}, \end{aligned}$$

$$\begin{aligned} E_X &:= \bar{E}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{P}_{\tau g} = R_{X_{max}}^T P_{Y\tau} R_{X_{max}} - R_{X_{min}}^T P_{Y\tau} R_{X_{min}}, \\ E_Y &:= \bar{P}_{Xg} \otimes \bar{E}_{Yg} \otimes \bar{P}_{\tau g} = R_{Y_{max}}^T P_{Y\tau} R_{Y_{max}} - R_{Y_{min}}^T P_{X\tau} R_{Y_{min}}, \\ E_\tau &:= \bar{P}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{E}_{\tau g} = R_{\tau_{max}}^T P_{XY} R_{\tau_{max}} - R_{\tau_{min}}^T P_{X\tau} R_{\tau_{min}}, \end{aligned}$$

$$\begin{aligned} P_{XY} &:= \bar{P}_{Xg} \otimes \bar{P}_{Yg}, & P_{Y\tau} &:= \bar{P}_{Yg} \otimes \bar{P}_{\tau g}, & P_{X\tau} &:= \bar{P}_{Xg} \otimes \bar{P}_{\tau g}, \\ R_{X_{min}} &:= \mathbf{t}_{L_{Xg}}^T \otimes \bar{I}_{Yg} \otimes \bar{I}_{\tau g}, & R_{Y_{min}} &:= \bar{I}_{Xg} \otimes \mathbf{t}_{L_{Yg}}^T \otimes \bar{I}_{\tau g}, & R_{\tau_{min}} &:= \bar{I}_{Xg} \otimes \bar{I}_{Yg} \otimes \mathbf{t}_{L_{\tau g}}^T, \\ R_{X_{max}} &:= \mathbf{t}_{R_{Xg}}^T \otimes \bar{I}_{Yg} \otimes \bar{I}_{\tau g}, & R_{Y_{max}} &:= \bar{I}_{Xg} \otimes \mathbf{t}_{R_{Yg}}^T \otimes \bar{I}_{\tau g}, & R_{\tau_{max}} &:= \bar{I}_{Xg} \otimes \bar{I}_{Yg} \otimes \mathbf{t}_{R_{\tau g}}^T, \\ P &:= \bar{P}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{P}_{\tau g}, & M_\tau &:= \bar{I}_{Xg} \otimes \bar{I}_{Yg} \otimes \bar{M}_{\tau g}. \end{aligned}$$

Next, we demonstrate that the above three dimensional CG operators are SBP operators. Using the properties of tensor products (4.20a), (4.20d), we have that

$$\begin{aligned} D_X &= \bar{D}_{Xg} \otimes \bar{I}_{Yg} \otimes \bar{I}_{\tau g} \\ &= \bar{P}_{Xg}^{-1} \bar{Q}_{Xg} \otimes \bar{I}_{Yg} \otimes \bar{I}_{\tau g} \\ &= \left(\bar{P}_{Xg}^{-1} \otimes \bar{P}_{Yg}^{-1} \otimes \bar{P}_{\tau g}^{-1} \right) (\bar{Q}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{P}_{\tau g}) \\ &= (\bar{P}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{P}_{\tau g})^{-1} (\bar{Q}_{Xg} \otimes \bar{P}_{Yg} \otimes \bar{P}_{\tau g}) \\ &= P^{-1} Q_X. \end{aligned} \quad (4.21)$$

To demonstrate that these operators mimic integration by parts, and therefore are SBP, first, recall the integration by parts formula for the X derivative in multiple dimensions for a hyperrectangle

$$\int_{\Omega} \mathcal{V} \frac{\partial \mathcal{U}}{\partial X} d\Omega + \int_{\Omega} \mathcal{U} \frac{\partial \mathcal{V}}{\partial X} d\Omega = \int_{\Gamma} \mathcal{V} \mathcal{U} n_X d\Gamma = \int_{Y=Y_{min}}^{Y_{max}} \int_{\tau=\tau_{min}}^{\tau_{max}} \mathcal{V} \mathcal{U}|_{X_{min}}^{X_{max}} d\tau dY, \quad (4.22)$$

where n_X is the X component of the outward facing unit normal on the boundary of Ω , i.e., $\Gamma := \partial\Omega$. Discretizing the LHS of (4.22) using the above operators results in

$$\begin{aligned} \mathbf{v}^T \mathbf{P} \mathbf{D}_X \mathbf{u} + \mathbf{u}^T \mathbf{P} \mathbf{D}_X \mathbf{v} &= \mathbf{v}^T \mathbf{Q}_X \mathbf{u} + \mathbf{u}^T \mathbf{Q}_X \mathbf{v} \\ &= \mathbf{v}^T \mathbf{Q}_X \mathbf{u} + (\mathbf{v}^T \mathbf{Q}_X^T \mathbf{u})^T \\ &= \mathbf{v}^T \mathbf{Q}_X \mathbf{u} + \mathbf{v}^T \mathbf{Q}_X^T \mathbf{u} \\ &= \mathbf{v}^T (\mathbf{Q}_X + \mathbf{Q}_X^T) \mathbf{u} \\ &= \mathbf{v}^T \left((\bar{\mathbf{Q}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{P}}_{\tau g}) + (\bar{\mathbf{Q}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{P}}_{\tau g})^T \right) \mathbf{u} \\ &= \mathbf{v}^T \left((\bar{\mathbf{Q}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{P}}_{\tau g}) + (\bar{\mathbf{Q}}_{Xg}^T \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{P}}_{\tau g}) \right) \mathbf{u} \\ &= \mathbf{v}^T \left((\bar{\mathbf{Q}}_{Xg} + \bar{\mathbf{Q}}_{Xg}^T) \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{P}}_{\tau g} \right) \mathbf{u} \\ &= \mathbf{v}^T (\bar{\mathbf{E}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{P}}_{\tau g}) \mathbf{u} \\ &= \mathbf{v}^T \mathbf{E}_X \mathbf{u} \\ &= \mathbf{v}^T (\mathbf{R}_{X_{max}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{max}} - \mathbf{R}_{X_{min}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{min}}) \mathbf{u}, \end{aligned} \quad (4.23)$$

where we have used the following properties of tensor products (4.20b) (4.20c). To understand why the RHS of (4.23) approximates the RHS of integration by parts (4.22), and therefore the operators are SBP, note that, for example, $\mathbf{R}_{X_{max}} \mathbf{u}$ results in a vector of $\mathcal{U}$ evaluated at the surface where $X = X_{max}$ and thus

$$\begin{aligned} \mathbf{v}^T \mathbf{R}_{X_{max}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{max}} \mathbf{u} &\approx \int_{Y=Y_{min}}^{Y_{max}} \int_{\tau=\tau_{min}}^{\tau_{max}} \mathcal{V}(X_{max}) \mathcal{U}(X_{max}) d\tau dY, \\ \mathbf{v}^T \mathbf{R}_{X_{min}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{min}} \mathbf{u} &\approx \int_{Y=Y_{min}}^{Y_{max}} \int_{\tau=\tau_{min}}^{\tau_{max}} \mathcal{V}(X_{min}) \mathcal{U}(X_{min}) d\tau dY. \end{aligned} \quad (4.24)$$

Next, we introduce an SBP operator that mimics integration by parts for the term $\frac{1}{4} \partial_{\tau}^{-1} \left(\frac{1}{G_x} \frac{\partial^2}{\partial X^2} + \frac{1}{G_y} \frac{\partial^2}{\partial Y^2} \right) \mathcal{P}$. For this purpose, recollect the definition of second derivative SBP operators 3.2.3, by taking advantage of the fact $\mathbf{D}_{\tau} \mathbf{M}_{\tau} \approx \mathbf{I}$ (see Figure 4.2), we define the modified second derivative as

$$\tilde{\mathbf{D}}_{2X} := \mathbf{P}^{-1} (-\mathbf{M}_{\tau}^T \mathbf{D}_{\tau}^T \mathbf{A}_X + \mathbf{E}_X \mathbf{D}_X), \quad (4.25)$$

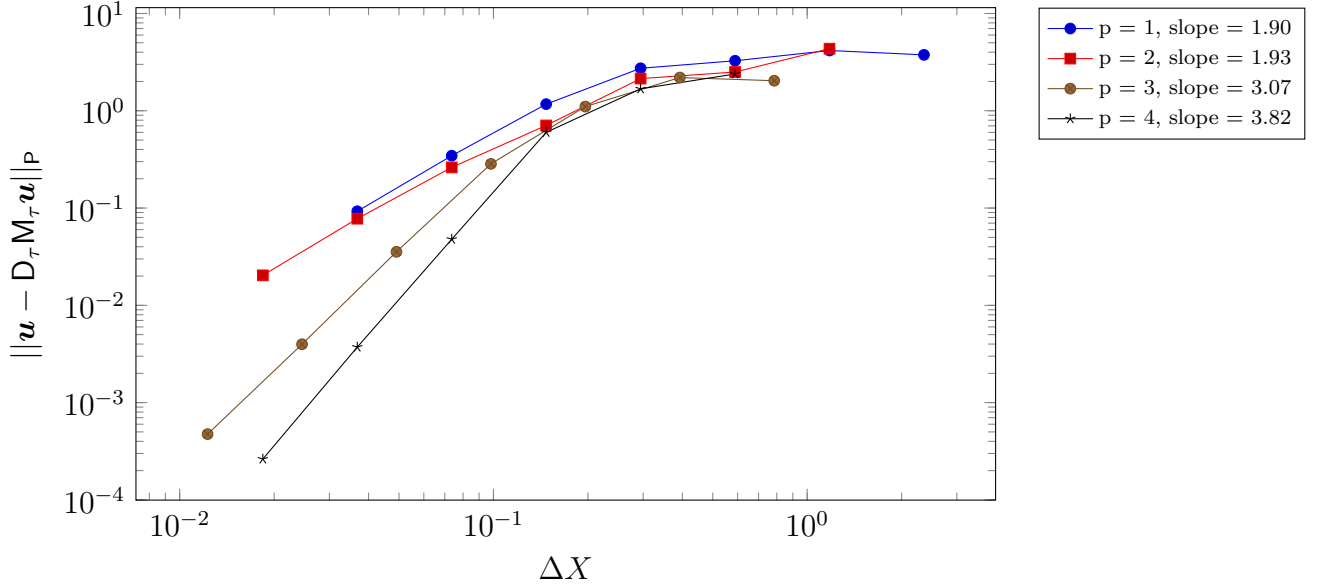


Figure 4.2: Convergence plot of the $D_\tau M_\tau u$ term. The domain is discretized using multiple elements and ΔX is computed by dividing the domain length in the X direction by the number of elements in the X direction. The coarsest mesh contains two elements while at each refinement level, the number of elements is doubled. The slopes are computed using the line of best fit through the last three data points.

thus,

$$\frac{\partial^2}{\partial X^2} \partial_\tau^{-1} \mathcal{P} \approx \tilde{D}_{2X} M_\tau \mathcal{P}. \quad (4.26)$$

Next, we show that this operator satisfies integration by parts, which for the term under consideration, is given as follows:

$$\int_\Omega \mathcal{P} \frac{\partial^2}{\partial X^2} \partial_\tau^{-1} \mathcal{P} = \int_\Gamma \mathcal{P} \frac{\partial}{\partial X} (\partial_\tau^{-1} \mathcal{P}) n_X d\Gamma - \int_\Omega \left(\frac{\partial \mathcal{P}}{\partial X} \right) \left(\frac{\partial}{\partial X} \partial_\tau^{-1} \mathcal{P} \right) d\Omega. \quad (4.27)$$

Hence, discretizing the LHS of (4.27) gives

$$\mathbf{p}^T \mathbf{P} \tilde{D}_{2Xg} M_\tau \mathbf{p} = \mathbf{p}^T \mathbf{E}_X D_X M_\tau \mathbf{p} - \mathbf{p}^T M_\tau^T D_\tau^T A_X M_\tau \mathbf{p}, \quad (4.28)$$

which mimics integration by parts. In order to see this, note that

$$\mathbf{u}^T \mathbf{E}_X \mathbf{v} \approx \int_\Gamma \mathcal{U} \mathcal{V} n_X d\Gamma, \quad \mathbf{u}^T \mathbf{A}_X \mathbf{v} \approx \int_\Omega \frac{\partial \mathcal{U}}{\partial X} \frac{\partial \mathcal{V}}{\partial X} d\Omega, \quad (4.29)$$

thus,

$$\begin{aligned}\mathbf{p}^T \mathbf{E}_X \mathbf{D}_X \mathbf{M}_\tau \mathbf{p} &\approx \int_\Gamma \mathcal{P} \frac{\partial}{\partial X} (\partial_\tau^{-1} \mathcal{P}) n_X d\Gamma, \\ \mathbf{p}^T \mathbf{A}_X \mathbf{M}_\tau \mathbf{p} &\approx \int_\Omega \left(\frac{\partial \mathcal{P}}{\partial X} \right) \left(\frac{\partial}{\partial X} \partial_\tau^{-1} \mathcal{P} \right) d\Omega.\end{aligned}\tag{4.30}$$

recall $\mathbf{D}_\tau \mathbf{M}_\tau \approx \mathbf{I}$, then we have

$$\mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_X \mathbf{M}_\tau \mathbf{p} \approx \int_\Omega \frac{\partial}{\partial \tau} \left(\partial_\tau^{-1} \frac{\partial \mathcal{P}}{\partial X} \right) \left(\partial_\tau^{-1} \frac{\partial \mathcal{P}}{\partial X} \right) d\Omega.\tag{4.31}$$

4.2.1 Semi Discrete Form of KZK Equation

We discretize the KZK equation (4.4) with our CG-SBP operators as follows:

$$\begin{aligned}& \frac{d\mathbf{p}}{d\sigma} - A \left(\frac{1}{3} \mathbf{D}_\tau [\mathbf{p}] \mathbf{p} + \frac{1}{3} [\mathbf{p}] \mathbf{D}_\tau \mathbf{p} \right) - \tilde{N} \mathbf{D}_{2\tau} \mathbf{p} - \frac{1}{G_y} \tilde{\mathbf{D}}_{2Y} \mathbf{M}_\tau \mathbf{p} - \frac{1}{G_x} \tilde{\mathbf{D}}_{2X} \mathbf{M}_\tau \mathbf{p} \\ &= A \left(s_1 \mathbf{P}^{-1} \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} [\mathbf{p}] \mathbf{p} + s_2 \mathbf{P}^{-1} \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} [\mathbf{p}] \mathbf{p} \right) \\ &+ \tilde{N} \left(s_3 \mathbf{P}^{-1} \mathbf{D}_\tau^T \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} \mathbf{p} + s_4 \mathbf{P}^{-1} \mathbf{D}_\tau^T \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} \mathbf{p} \right) \\ &+ \frac{1}{G_y} \left(s_5 \mathbf{P}^{-1} \mathbf{R}_{Y_{min}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{min}} \mathbf{D}_Y \mathbf{M}_\tau \mathbf{p} + s_6 \mathbf{P}^{-1} \mathbf{M}_\tau^T \mathbf{D}_Y^T \mathbf{R}_{Y_{max}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{max}} \mathbf{p} \right) \\ &+ \frac{1}{G_x} \left(s_7 \mathbf{P}^{-1} \mathbf{R}_{X_{min}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{min}} \mathbf{D}_X \mathbf{M}_\tau \mathbf{p} + s_8 \mathbf{P}^{-1} \mathbf{M}_\tau^T \mathbf{D}_X^T \mathbf{R}_{X_{max}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{max}} \mathbf{p} \right),\end{aligned}\tag{4.32}$$

where the SATs are given as

$$\begin{aligned}\mathbf{SAT}_L &:= \underbrace{A s_1 \mathbf{P}^{-1} \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} [\mathbf{p}] \mathbf{p}}_I + \underbrace{\tilde{N} s_3 \mathbf{P}^{-1} \mathbf{D}_\tau^T \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} \mathbf{p}}_{II} \\ &+ \underbrace{\frac{1}{G_y} s_5 \mathbf{P}^{-1} \mathbf{R}_{Y_{min}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{min}} \mathbf{D}_Y \mathbf{M}_\tau \mathbf{p}}_{III} + \underbrace{\frac{1}{G_x} s_7 \mathbf{P}^{-1} \mathbf{R}_{X_{min}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{min}} \mathbf{D}_X \mathbf{M}_\tau \mathbf{p}}_{IV}, \\ \mathbf{SAT}_R &:= \underbrace{A s_2 \mathbf{P}^{-1} \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} [\mathbf{p}] \mathbf{p}}_V + \underbrace{\tilde{N} s_4 \mathbf{P}^{-1} \mathbf{D}_\tau^T \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} \mathbf{p}}_{VI} \\ &+ \underbrace{\frac{1}{G_y} s_6 \mathbf{P}^{-1} \mathbf{M}_\tau^T \mathbf{D}_Y^T \mathbf{R}_{Y_{max}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{max}} \mathbf{p}}_{VII} + \underbrace{\frac{1}{G_x} s_8 \mathbf{P}^{-1} \mathbf{M}_\tau^T \mathbf{D}_X^T \mathbf{R}_{X_{max}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{max}} \mathbf{p}}_{VIII},\end{aligned}\tag{4.33}$$

and $s_1, \dots, s_8$ are SAT parameters that will be specified to obtain stability. The LHS of (4.32) is a discretization of the KZK equation while the RHS of (4.32) are the SATs used to weakly impose the boundary conditions. Note that we have discretized the Burgers' term and the second derivative term for τ as in Chapter 3. Similarly, the SAT terms are built based upon the previously presented discretizations, where I , II , V , and VI impose homogeneous Dirichlet boundary conditions in the τ direction (I and II at τ_{min} while V and VI at τ_{max}). Based on the same idea for constructing the SATs for the linear diffusion equation (3.64), III imposes a homogeneous Neumann boundary condition on the $X - \tau$ plane at Y_{min} , while term IV impose a homogeneous Neumann boundary conditions on the $Y - \tau$ plane at Y_{min} . Finally, VII and $VIII$ impose homogeneous Dirichlet boundary conditions at X_{max} and Y_{max} , respectively. The next theorem proves stability of (4.32).

Theorem 4.2.1. *The semi discrete form of the KZK equation (4.32) is stable if $s_1 = \frac{1}{3}$, $s_2 = -\frac{1}{3}$, $s_3 = 1$, $s_4 = -1$, $s_5 = 1$, $s_6 = -1$, $s_7 = 1$, $s_8 = -1$.*

Proof. We first rewrite (4.32) as

$$\begin{aligned}
\frac{d\mathbf{p}}{d\sigma} = & A \left(\frac{1}{3} D_\tau [\mathbf{p}] \mathbf{p} + \frac{1}{3} [\mathbf{p}] D_\tau \mathbf{p} + s_1 \mathbf{P}^{-1} \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} [\mathbf{p}] \mathbf{p} + s_2 \mathbf{P}^{-1} \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} [\mathbf{p}] \mathbf{p} \right) \\
& + \tilde{N} (D_{2\tau} \mathbf{p} + s_3 \mathbf{P}^{-1} D_\tau^T \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} \mathbf{p} + s_4 \mathbf{P}^{-1} D_\tau^T \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} \mathbf{p}) \\
& + \frac{1}{G_y} (\tilde{D}_{2Y} \mathbf{M}_\tau \mathbf{p} + s_5 \mathbf{P}^{-1} \mathbf{R}_{Yg}^T \mathbf{P}_{X\tau} \mathbf{R}_{Yg} D_Y \mathbf{M}_\tau \mathbf{p} + s_6 \mathbf{P}^{-1} \mathbf{M}_\tau^T D_Y^T \mathbf{R}_{Y_{max}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{max}} \mathbf{p}) \\
& + \frac{1}{G_x} (\tilde{D}_{2X} \mathbf{M}_\tau \mathbf{p} + s_7 \mathbf{P}^{-1} \mathbf{R}_{X_{min}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{min}} D_X \mathbf{M}_\tau \mathbf{p} + s_8 \mathbf{P}^{-1} \mathbf{M}_\tau^T D_X^T \mathbf{R}_{X_{max}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{max}} \mathbf{p}).
\end{aligned} \tag{4.34}$$

Multiplying (4.34) by $\mathbf{p}^T \mathbf{P}$, we obtain

$$\begin{aligned}
\mathbf{p}^T \mathbf{P} \frac{d\mathbf{p}}{d\sigma} = & \underbrace{A \left(\frac{1}{3} \mathbf{p}^T \mathbf{Q}_\tau [\mathbf{p}] \mathbf{p} + \frac{1}{3} \mathbf{p} \mathbf{Q}_\tau^T [\mathbf{p}] \mathbf{p} + s_1 \mathbf{p}^T \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} [\mathbf{p}] \mathbf{p} + s_2 \mathbf{p}^T \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} [\mathbf{p}] \mathbf{p} \right)}_{I:=} \\
& + \underbrace{\tilde{N} \left(\mathbf{p}^T (-\mathbf{A}_\tau + \mathbf{E}_\tau \mathbf{D}_\tau) \mathbf{p} + s_3 \mathbf{p}^T \mathbf{D}_\tau^T \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} \mathbf{p} + s_4 \mathbf{p}^T \mathbf{D}_\tau^T \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} \mathbf{p} \right)}_{II:=} \\
& + \underbrace{\frac{1}{G_y} (\mathbf{p}^T (-\mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_Y + \mathbf{E}_Y \mathbf{D}_Y) \mathbf{M}_\tau \mathbf{p})}_{III:=} \\
& + \underbrace{s_5 \mathbf{p}^T \mathbf{R}_{Yg}^T \mathbf{P}_{X\tau} \mathbf{R}_{Yg} \mathbf{D}_Y \mathbf{M}_\tau \mathbf{p} + s_6 \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_Y^T \mathbf{R}_{Y_{max}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{max}} \mathbf{p}}_{IV:=} \\
& + \underbrace{\frac{1}{G_x} (\mathbf{p}^T (-\mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_X + \mathbf{E}_X \mathbf{D}_X) \mathbf{M}_\tau \mathbf{p})}_{IV:=} \\
& + \underbrace{s_7 \mathbf{p}^T \mathbf{R}_{X_{min}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{min}} \mathbf{D}_X \mathbf{M}_\tau \mathbf{p} + s_8 \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_X^T \mathbf{R}_{X_{max}}^T \mathbf{P}_{Y\tau} \mathbf{R}_{X_{max}} \mathbf{p}}_{IV:=}.
\end{aligned} \tag{4.35}$$

To simplify the discussion, we will examine the volume terms and associated SATs in (4.35) one term at a time. First, consider the Burgers' term I . Since $\mathbf{Q}_\tau + \mathbf{Q}_\tau^T = \mathbf{E}_\tau = \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} - \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}}$, combining similar terms and using $s_1 = \frac{1}{3}$ and $s_2 = -\frac{1}{3}$, this term reduces as follows:

$$\begin{aligned}
I &= A \left(\frac{1}{3} \mathbf{p}^T (\mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} - \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}}) [\mathbf{p}] \mathbf{p} + s_1 \mathbf{p}^T \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} [\mathbf{p}] \mathbf{p} + \right. \\
& \quad \left. s_2 \mathbf{p}^T \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} [\mathbf{p}] \mathbf{p} \right) \\
&= A \left(\left(-\frac{1}{3} + s_1 \right) \mathbf{p}^T \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} [\mathbf{p}] \mathbf{p} + \left(\frac{1}{3} + s_2 \right) \mathbf{p}^T \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} [\mathbf{p}] \mathbf{p} \right) \\
&= 0.
\end{aligned} \tag{4.36}$$

Next, recall that $\mathbf{E}_\tau = \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} - \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}}$, then second derivative term in τ

(term *II*) with its SATs reduces as follows:

$$\begin{aligned}
II &= \tilde{N}(-\mathbf{p}^T \mathbf{A}_\tau \mathbf{p} + \mathbf{p}^T (\mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} - \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}}) \mathbf{D}_\tau \mathbf{p} \\
&\quad + s_3 \mathbf{p}^T \mathbf{D}_\tau^T \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} \mathbf{p} + s_4 \mathbf{p}^T \mathbf{D}_\tau^T \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} \mathbf{p}) \\
&= \tilde{N}(-\mathbf{p}^T \mathbf{A}_\tau \mathbf{p} + (1 + s_4) \mathbf{p}^T \mathbf{R}_{\tau_{max}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{max}} \mathbf{p} + (-1 + s_3) \mathbf{p}^T \mathbf{D}_\tau^T \mathbf{R}_{\tau_{min}}^T \mathbf{P}_{XY} \mathbf{R}_{\tau_{min}} \mathbf{p}) \\
&= -\tilde{N} \mathbf{p}^T \mathbf{A}_\tau \mathbf{p},
\end{aligned} \tag{4.37}$$

where to obtain the last equality we set $s_3 = 1$ and $s_4 = -1$.

Next, we consider the modified second derivative term with respect to Y (term *III*) and its SAT terms. Since $\mathbf{E}_Y = \mathbf{R}_{Y_{max}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{max}} - \mathbf{R}_{Y_g}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_g}$, then we combine the same terms such that

$$\begin{aligned}
III &= \frac{1}{G_y} (\mathbf{p}^T (-\mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_Y + (\mathbf{R}_{Y_{max}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{max}} - \mathbf{R}_{Y_g}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_g}) \mathbf{D}_Y) \mathbf{M}_\tau \mathbf{p} \\
&\quad + s_5 \mathbf{p}^T \mathbf{R}_{Y_g}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_g} \mathbf{D}_Y \mathbf{M}_\tau \mathbf{p} + s_6 \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_Y^T \mathbf{R}_{Y_{max}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{max}} \mathbf{p}) \\
&= \frac{1}{G_y} (-\mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_Y \mathbf{M}_\tau \mathbf{p} + (-1 + s_5) \mathbf{p}^T \mathbf{R}_{Y_g}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_g} \mathbf{D}_Y \mathbf{M}_\tau \mathbf{p} \\
&\quad + (s_6 + 1) \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_Y^T \mathbf{R}_{Y_{max}}^T \mathbf{P}_{X\tau} \mathbf{R}_{Y_{max}} \mathbf{p}) \\
&= -\frac{1}{G_y} \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_Y \mathbf{M}_\tau \mathbf{p}.
\end{aligned} \tag{4.38}$$

An identical analysis of the second derivative term for X and its SATs results in

$$IV = -\frac{1}{G_x} \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_X \mathbf{M}_\tau \mathbf{p}. \tag{4.39}$$

The last term we need to deal with is $\mathbf{p}^T \mathbf{P} \frac{d}{d\sigma} \mathbf{p}$, where applying the chain rule results in

$$\mathbf{p}^T \mathbf{P} \frac{d}{d\sigma} \mathbf{p} = \frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p}. \tag{4.40}$$

Now we combine (4.36), (4.37), (4.38), (4.39), and (4.40) to obtain

$$\frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} = -\tilde{N} \mathbf{p}^T \mathbf{A}_\tau \mathbf{p} - \frac{1}{G_y} \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_Y \mathbf{M}_\tau \mathbf{p} - \frac{1}{G_x} \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_X \mathbf{M}_\tau \mathbf{p}. \tag{4.41}$$

Recall that $\mathbf{A}_\tau$ is a positive semi-definite matrix and $\tilde{N}$ is a positive constant, thus, $\tilde{N} \mathbf{p}^T \mathbf{A}_\tau \mathbf{p} \geq 0$, and therefore

$$\frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq -\frac{1}{G_y} \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_Y \mathbf{M}_\tau \mathbf{p} - \frac{1}{G_x} \mathbf{p}^T \mathbf{M}_\tau^T \mathbf{D}_\tau^T \mathbf{A}_X \mathbf{M}_\tau \mathbf{p}. \tag{4.42}$$

In this thesis, we only considered the case $\mathbf{A}_X = \sum_{i=1}^N \mathbf{R}_i^T \bar{\mathbf{D}}_X^T \bar{\mathbf{P}}_X \bar{\mathbf{D}}_X \mathbf{R}_i$ and $\mathbf{A}_Y = \sum_{i=1}^N \mathbf{R}_i^T \bar{\mathbf{D}}_Y^T \bar{\mathbf{P}}_Y \bar{\mathbf{D}}_Y \mathbf{R}_i$, let $\mathbf{v} := \mathbf{M}_\tau \mathbf{p}$, then (4.42) can be rewritten as follows:

$$\frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq -\frac{1}{G_x} \mathbf{v}^T \mathbf{D}_\tau^T \mathbf{A}_X \mathbf{v} - \frac{1}{G_y} \mathbf{v}^T \mathbf{D}_\tau^T \mathbf{A}_Y \mathbf{v}, \quad (4.43)$$

Using the definition of $\mathbf{D}_\tau, \mathbf{A}_X, \mathbf{A}_Y$, (4.41) can be expanded as

$$\begin{aligned} \frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq & -\frac{1}{G_x} \mathbf{v}^T \left(\bar{\mathbf{I}}_{Xg} \otimes \bar{\mathbf{I}}_{Yg} \otimes \bar{\mathbf{D}}_{\tau g}^T \right) \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{P}}_{\tau g} \right) \mathbf{v} \\ & -\frac{1}{G_y} \mathbf{v}^T \left(\bar{\mathbf{I}}_{Xg} \otimes \bar{\mathbf{I}}_{Yg} \otimes \bar{\mathbf{D}}_{\tau g}^T \right) \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{P}}_{\tau g} \right) \mathbf{v}. \end{aligned} \quad (4.44)$$

Note that $\bar{\mathbf{D}}_{\tau g} = \bar{\mathbf{P}}_{\tau g}^{-1} \bar{\mathbf{Q}}_{\tau g}$, thus, using the properties of tensor products (4.44) simplifies to

$$\frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq -\frac{1}{G_x} \mathbf{v}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g}^T \right) \mathbf{v} - \frac{1}{G_y} \mathbf{v}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g}^T \right) \mathbf{v}. \quad (4.45)$$

Next, we split the RHS of (4.45) to obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq & -\frac{1}{2G_x} \mathbf{v}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g}^T \right) \mathbf{v} - \frac{1}{2G_x} \mathbf{v}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g}^T \right) \mathbf{v} \\ & -\frac{1}{2G_y} \mathbf{v}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g}^T \right) \mathbf{v} - \frac{1}{2G_y} \mathbf{v}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g}^T \right) \mathbf{v}. \end{aligned} \quad (4.46)$$

Then, we take transpose of the second and fourth terms of (4.46), which results in

$$\begin{aligned} \frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq & -\frac{1}{2G_x} \mathbf{v}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g}^T \right) \mathbf{v} - \frac{1}{2G_x} \mathbf{v}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g} \right) \mathbf{v} \\ & -\frac{1}{2G_y} \mathbf{v}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g}^T \right) \mathbf{v} - \frac{1}{2G_y} \mathbf{v}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{Q}}_{\tau g} \right) \mathbf{v}. \end{aligned} \quad (4.47)$$

Using the property of tensor product and $\bar{\mathbf{Q}}_{\tau g} + \bar{\mathbf{Q}}_{\tau g}^T = \bar{\mathbf{E}}_{\tau g}$ on (4.47), gives that

$$\frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq -\frac{1}{2G_x} \mathbf{v}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{E}}_{\tau g} \right) \mathbf{v} - \frac{1}{2G_y} \mathbf{v}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{E}}_{\tau g} \right) \mathbf{v}. \quad (4.48)$$

Next, we substitute the definition of $\mathbf{v}$ back in (4.43) and then substituting the definition of $\mathbf{M}_\tau$ results in

$$\begin{aligned} \frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq & -\frac{1}{2G_x} \mathbf{p}^T \left(\bar{\mathbf{I}}_{Xg} \otimes \bar{\mathbf{I}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \right) \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{E}}_{\tau g} \right) \left(\bar{\mathbf{I}}_{Xg} \otimes \bar{\mathbf{I}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p} \\ & -\frac{1}{2G_y} \mathbf{p}^T \left(\bar{\mathbf{I}}_{Xg} \otimes \bar{\mathbf{I}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \right) \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{E}}_{\tau g} \right) \left(\bar{\mathbf{I}}_{Xg} \otimes \bar{\mathbf{I}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p}. \end{aligned} \quad (4.49)$$

Using the property (4.20d) of tensor products, (4.49) can be simplified as

$$\begin{aligned} \frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq & -\frac{1}{2G_x} \mathbf{p}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \bar{\mathbf{E}}_{\tau g} \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p} \\ & -\frac{1}{2G_y} \mathbf{p}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \bar{\mathbf{E}}_{\tau g} \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p}. \end{aligned} \quad (4.50)$$

Recall that $\bar{\mathbf{E}}_{\tau g} = \mathbf{t}_{R\tau g} \mathbf{t}_{R\tau g}^T - \mathbf{t}_{L\tau g} \mathbf{t}_{L\tau g}^T$, and then using the property (4.20d) of tensor product to obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq & -\frac{1}{2G_x} \mathbf{p}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \mathbf{t}_{R\tau g} \mathbf{t}_{R\tau g}^T \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p} + \frac{1}{2G_x} \mathbf{p}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \mathbf{t}_{L\tau g} \mathbf{t}_{L\tau g}^T \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p} \\ & -\frac{1}{2G_y} \mathbf{p}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \mathbf{t}_{R\tau g} \mathbf{t}_{R\tau g}^T \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p} + \frac{1}{2G_y} \mathbf{p}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \mathbf{t}_{L\tau g} \mathbf{t}_{L\tau g}^T \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p}. \end{aligned} \quad (4.51)$$

Next, since 1) $\bar{\mathbf{A}}_{Xg}$ and $\bar{\mathbf{A}}_{Yg}$ are positive semi-definite, 2) $\bar{\mathbf{P}}_{Xg}$ and $\bar{\mathbf{P}}_{Yg}$ are positive definite, and 3) $\bar{\mathbf{M}}_{\tau g}^T \mathbf{t}_{L\tau g} \mathbf{t}_{L\tau g}^T \bar{\mathbf{M}}_{\tau g} = \left(\mathbf{t}_{L\tau g}^T \bar{\mathbf{M}}_{\tau g} \right)^T \left(\mathbf{t}_{L\tau g}^T \bar{\mathbf{M}}_{\tau g} \right)$ is positive semi-definite, then we can drop the negative semi-definite term to obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq & \frac{1}{2G_x} \mathbf{p}^T \left(\bar{\mathbf{A}}_{Xg} \otimes \bar{\mathbf{P}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \mathbf{t}_{L\tau g} \mathbf{t}_{L\tau g}^T \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p} \\ & + \frac{1}{2G_y} \mathbf{p}^T \left(\bar{\mathbf{P}}_{Xg} \otimes \bar{\mathbf{A}}_{Yg} \otimes \bar{\mathbf{M}}_{\tau g}^T \mathbf{t}_{L\tau g} \mathbf{t}_{L\tau g}^T \bar{\mathbf{M}}_{\tau g} \right) \mathbf{p}. \end{aligned} \quad (4.52)$$

Since the entries of $\mathbf{t}_{L\tau g}^T$ are 0s except the first entry and the first row of $\bar{\mathbf{M}}_{\tau g}$ is all 0s, then $\mathbf{t}_{L\tau g}^T \bar{\mathbf{M}}_{\tau g}$ is a zero matrix, which indicates $\bar{\mathbf{M}}_{\tau g}^T \mathbf{t}_{L\tau g} \mathbf{t}_{L\tau g}^T \bar{\mathbf{M}}_{\tau g}$ is a zero matrix as well, then by the properties of tensor products, we have that

$$\frac{1}{2} \frac{d}{d\sigma} \mathbf{p}^T \mathbf{P} \mathbf{p} \leq 0. \quad (4.53)$$

Then, integrating (4.53) in σ and rearranging gives

$$\|\mathbf{p}(\sigma_{max})\|_{\mathbf{P}}^2 \leq \|\mathbf{p}_0\|^2, \quad (4.54)$$

where $\mathbf{p}_0$ is a vector constructed from evaluating the source condition on the mesh nodes and $\|\mathbf{v}\|_{\mathbf{P}}^2 := \mathbf{v}^T \mathbf{P} \mathbf{v}$. Thus, the discretization is stable.

□

4.3 Chapter Summary

In this chapter, we derived a non-dimensional form of the KZK equation that we then prove is stable under two sets of boundary conditions. Next, we extended our global one-dimensional CG SBP operators to multiple dimensions using tensor products and demonstrated that the resulting operators are SBP. Moreover, we developed a modified second derivative term key in constructing the proposed schemes. Finally, we proved that the resulting semi-discrete form is stable under the two options for the second derivative in τ that are considered in this thesis. In the next chapter, we present numerical experiments to demonstrate the accuracy properties of the proposed scheme as well as some HIFU test cases.

Chapter 5

Numerical Results

In this chapter, we characterize the accuracy of the proposed schemes for the KZK equation as well as numerical verification of the stability properties of the scheme. Finally, we apply the scheme to a case related to HIFU.

5.1 Accuracy of the CG-SBP-SAT Discretization

In this section, we numerically characterize the accuracy and stability properties of the proposed scheme. For this purpose, we use the method of manufactured solutions [90], specifically $\mathcal{P}_{MMS} = \cos(X)\cos(Y)\sin(\tau)e^{-\sigma}$ is used to determine the convergence rates of the scheme. Note that σ is taken as the artificial temporal variable and we use RK4 to time march on this variable. We consider the following KZK problem:

$$\begin{aligned} \frac{\partial \mathcal{P}}{\partial \sigma} - NP \frac{\partial \mathcal{P}}{\partial \tau} - A \frac{\partial^2 \mathcal{P}}{\partial \tau^2} - \frac{1}{4} \partial_\tau^{-1} \left(\frac{1}{G_x} \frac{\partial^2}{\partial X^2} + \frac{1}{G_y} \frac{\partial^2}{\partial Y^2} \right) \mathcal{P} &= \mathcal{F}(X, Y, \tau, \sigma), \\ (X, Y, \tau) &\in \left[0, \frac{3\pi}{2}\right] \times \left[0, \frac{3\pi}{2}\right] \times [0, \pi], \end{aligned} \quad (5.1)$$

where

$$\begin{aligned} \mathcal{F}(X, Y, \tau, \sigma) &= -\cos(Y)\cos(X)\sin(\tau)e^{-\sigma} - N\cos^2(Y)\cos^2(X)\sin(\tau)(e^{-\sigma})^2\cos(\tau) \\ &\quad + A\cos(Y)\cos(X)\sin(\tau)e^{-\sigma} - \frac{\cos(X)\cos(Y)e^{-\sigma}(G_x\cos(\tau) + G_y\cos(\tau) - G_x - G_y)}{4G_xG_y} \end{aligned} \quad (5.2)$$

is the forcing term due to the manufacture solution. In the convergence study, we pick the coefficients as

$$N = 0.1, \quad A = 1, \quad G_x = G_y = 5. \quad (5.3)$$

In order to reduce the computational cost of simulations, we will only consider the boundary conditions for the axisymmetric problem, i.e., (4.9) mentioned in the previous chapter; thus, the boundary conditions for the convergence study are

$$\begin{aligned} \mathcal{P}(X, Y, 0, \sigma) &= 0, & \mathcal{P}(X, Y, \pi, \sigma) &= 0, \\ \frac{\partial \mathcal{P}}{\partial X}(0, Y, \tau, \sigma) &= 0, & \mathcal{P}\left(\frac{3\pi}{2}, Y, \tau, \sigma\right) &= 0, \\ \frac{\partial \mathcal{P}}{\partial Y}(X, 0, \tau, \sigma) &= 0, & \mathcal{P}\left(X, \frac{3\pi}{2}, \tau, \sigma\right) &= 0. \end{aligned} \quad (5.4)$$

Based on $\mathcal{P}_{MMS}$, the source condition is

$$\mathcal{P} = \cos(X) \cos(Y) \sin(\tau), \quad \sigma = 0. \quad (5.5)$$

The convergence rates of numerical solution are given in Figure 5.1 and we find that the convergence rate is at least $p + 1$.

At a high level, we can consider our semi-discrete form as the following ODE:

$$\frac{d\mathbf{p}}{d\sigma} = \mathbf{RHS}(\mathbf{p}) + \mathbf{f}, \quad (5.6)$$

where our discretization of the spatial terms is generically represented by $\mathbf{RHS}(\mathbf{p})$ and $\mathbf{f}$ is the evaluation of the source term $\mathcal{F}$ from the method of manufacture solutions. Our stability proof, Theorem 4.2.1, demonstrates that

$$\mathbf{p}^T \mathbf{P} \mathbf{RHS}(\mathbf{p}) \leq 0, \quad (5.7)$$

which gives us a means of numerically demonstrating stability of the semi-discrete form. In Figure 5.2, we show that $\mathbf{p}^T \mathbf{P} \mathbf{RHS}(\mathbf{p}) \leq 0$ is satisfied.

5.2 Application of the CG-SBP-SAT Discretization to HIFU

To demonstrate the application of the proposed scheme to HIFU, we consider a similar problem to that in [55]. Recall the physical meaning of the independent variables involved

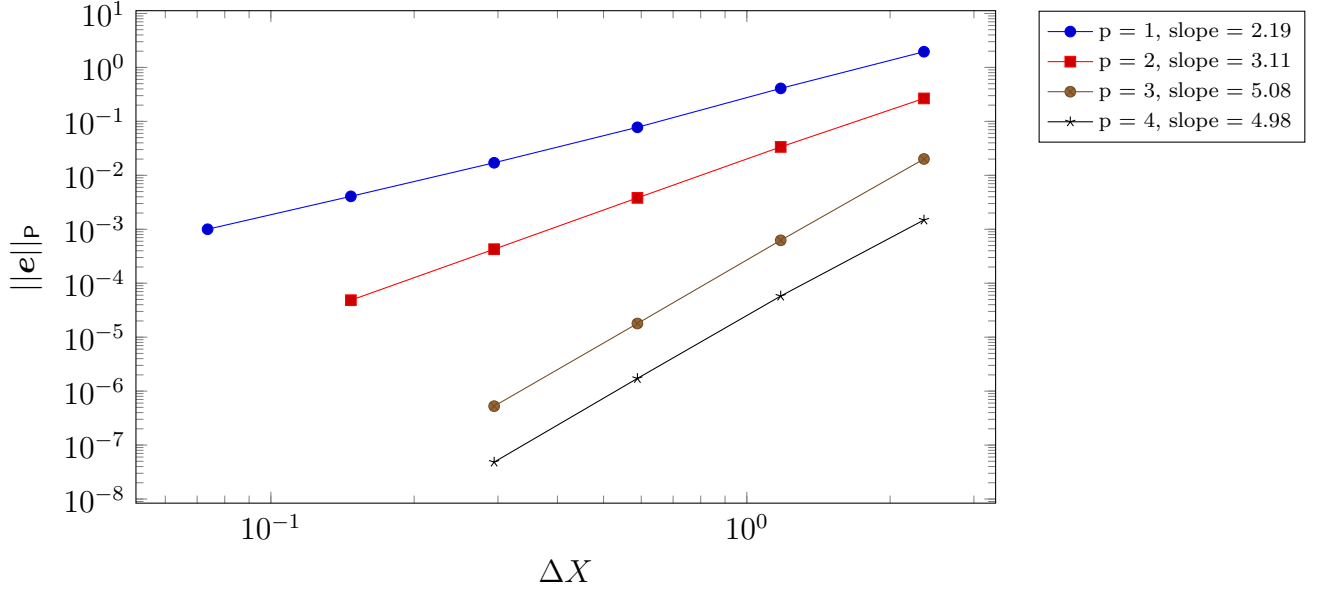


Figure 5.1: Convergence plot of the KZK equation discretized using CG SBP-SAT method, with the boundary conditions (5.4) and the initial condition (5.5). The domain is discretized using multiple elements and ΔX is computed by dividing the domain length in the X direction by the number of elements in the X direction. The coarsest mesh contains two elements while at each refinement level, the number of elements is doubled. The slopes are computed using the line of best fit through the last three data points.

in the KZK equation, X and Y are the space variables, and σ represents the wave propagation direction. Here, the minimum σ_{min} and the maximum σ_{max} of σ is set to be 0 and 1, respectively. More precisely, σ_{min} is the original location of the source excitation and σ_{max} is the final targeted position. The domain of X and Y must be chosen large enough such that the magnitude of reflected waves, which can deteriorate the accuracy of the numerical results, is sufficiently small [55]. During the numerical computation, the domain of X and Y is chosen as $X \in [0, 4]$, $Y \in [0, 4]$, which satisfies the criterion for the focused piston source suggested in [55] which is the problem we are solving in this section. It is crucial to choose a sufficiently large time window to encompass the whole waveform [55]. In the numerical simulation, $\tau = [-10\pi, 24\pi]$ is chosen as the time window based on the recommendation in [55]. Recall, the general form of the source condition (4.6) mentioned in the previous chapter, here we choose $G_{xs} = G_{ys} = 5$ for the numerical simulation. More precisely, the source condition is

$$\mathcal{P} = \mathcal{F}(\tau + G_{xs}\mathbf{X}^2 + G_{ys}\mathbf{Y}^2)\mathcal{G}(\mathbf{X}, \mathbf{Y}) \quad \text{at } \sigma = 0 \quad (5.8)$$

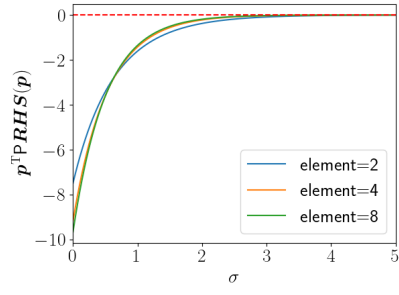
where

$$\mathcal{G}(\mathbf{X}, \mathbf{Y}) = \begin{cases} 1 & 0 \leq \mathbf{X} \leq 1 \quad \text{and} \quad 0 \leq \mathbf{Y} \leq 1, \\ 0 & \text{otherwise,} \end{cases} \quad (5.9)$$

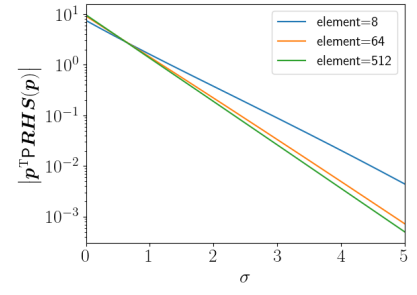
$$\mathcal{F}(\tau + G_{xs}\mathbf{X}^2 + G_{ys}\mathbf{Y}^2) = e^{-\left(\frac{\omega_0(\tau + G_{xs}\mathbf{X}^2 + G_{ys}\mathbf{Y}^2)}{3}\right)^2} \sin(\omega_0(\tau + G_{xs}\mathbf{X}^2 + G_{ys}\mathbf{Y}^2)), \quad (5.10)$$

where ω_0 is the frequency of the wave. As in the previous section, we consider the axisymmetric problem and therefore use boundary conditions (4.9). In this thesis, we try to match the numerical results in [55], but could not determine their choice for w_0 . During the numerical experiments, we set $w_0 = 1$ and instead look to match the general patterns observed in [55]. We time march in the σ direction using RK4 for $\sigma = 0$ to $\sigma = 1$, with a time step of 10^{-5} . The three-dimensional numerical pressure plots are shown in the Figure 5.3. and demonstrate that the pressure from the ultrasound beam gradually focuses as σ tends to $\sigma = 1$, as expected.

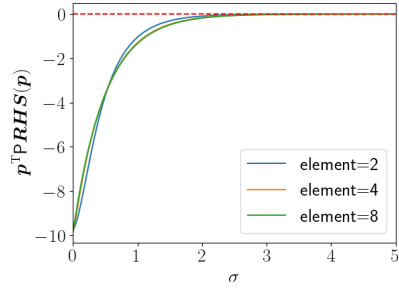
In addition, Figure 5.4 shows the pressure profile of the ultrasound beams at $X = 0$, and $Y = 0$. Note that the focal point of the HIFU is at $(X, Y, \tau) = (0, 0, 0)$ and we see from the figure that as σ increases the magnitude of the pressure around this point increases reaching a maximum at $\sigma = 1$, as expected. Figure 5.5 shows the envelop of the pressure, which similarly demonstrates the focusing of the pressure at the origin.



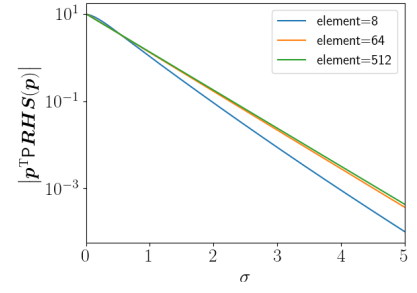
(a) $p = 1$



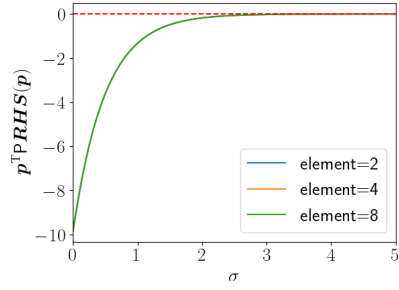
(b) $p = 1$



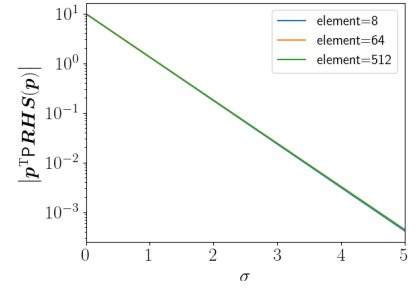
(c) $p = 2$



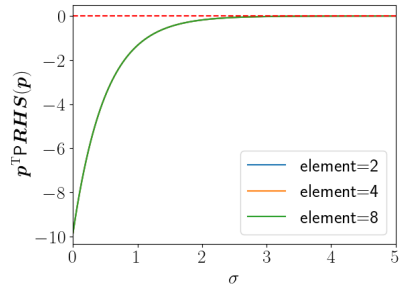
(d) $p = 2$



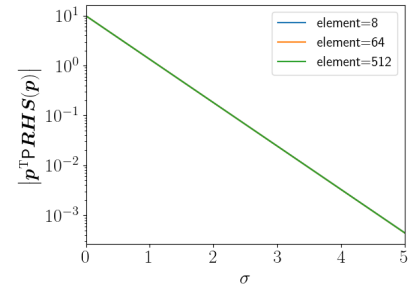
(e) $p = 3$



(f) $p = 3$

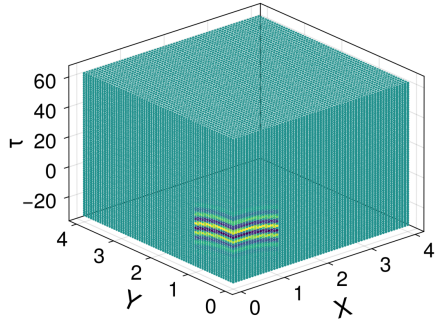


(g) $p = 4$

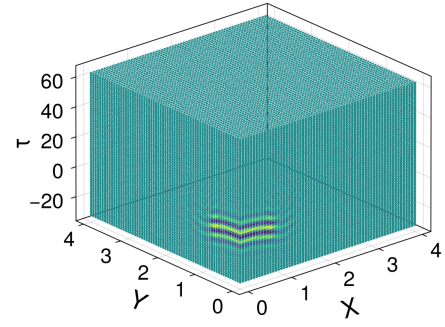


(h) $p = 4$

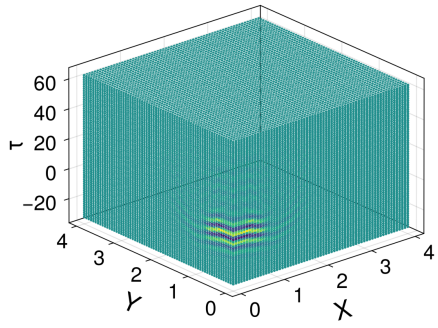
Figure 5.2: Plot of $\mathbf{p}^T \mathbf{RHS}(\mathbf{p})$ versus σ for degree $p = 1, \dots, 4$ discretizations on meshes with 8, 64, and 512 elements. Graphs on the right are use a logarithmic y -axis.



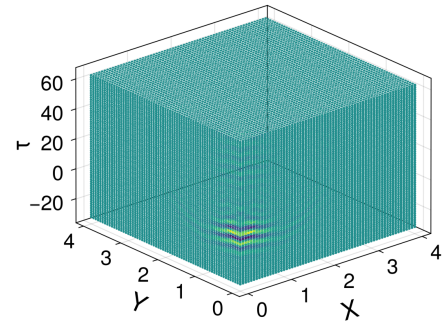
(a) $\sigma = 0.0$



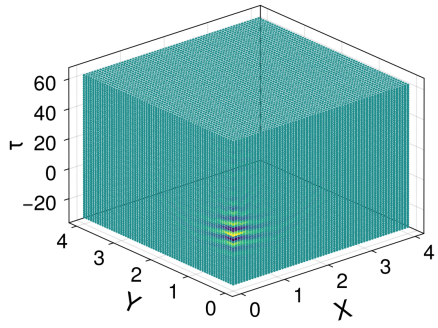
(b) $\sigma = 0.2$



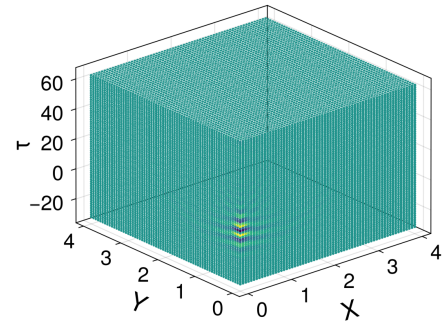
(c) $\sigma = 0.4$



(d) $\sigma = 0.6$

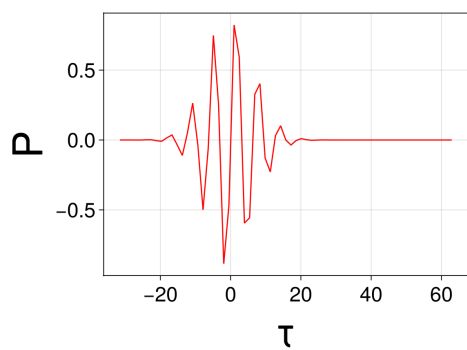


(e) $\sigma = 0.8$

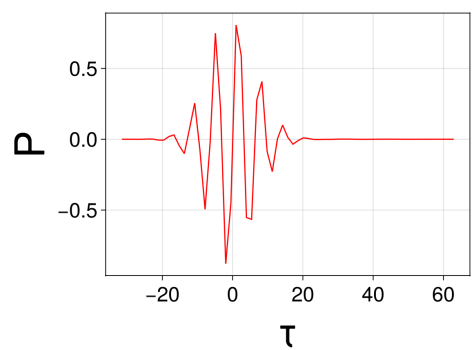


(f) $\sigma = 1.0$

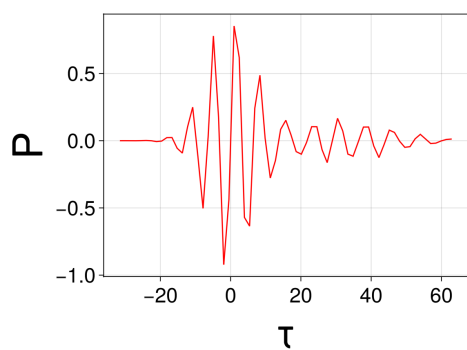
Figure 5.3: Ultrasound visualization



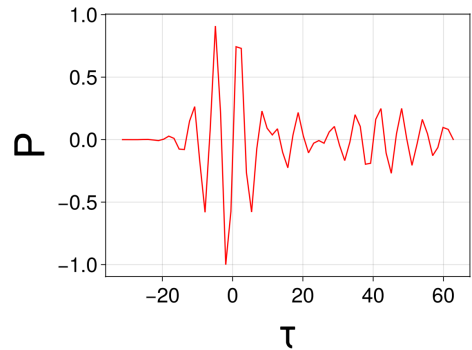
(a) $\sigma = 0.0$



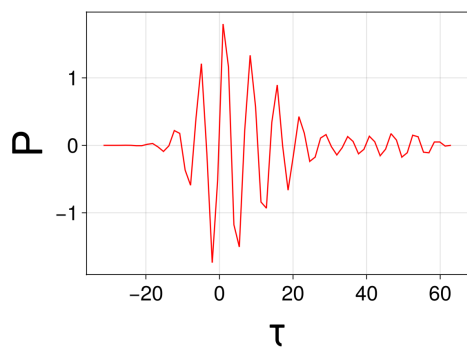
(b) $\sigma = 0.2$



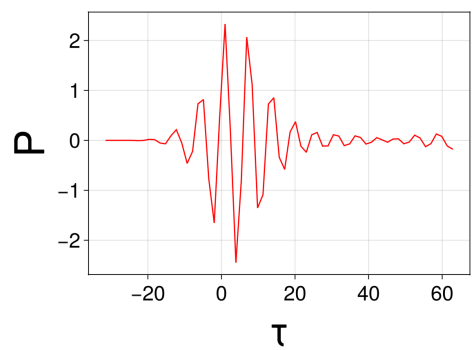
(c) $\sigma = 0.4$



(d) $\sigma = 0.6$

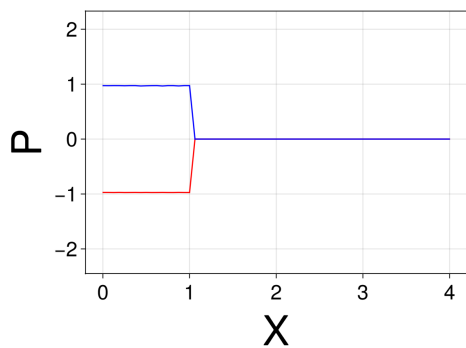


(e) $\sigma = 0.8$

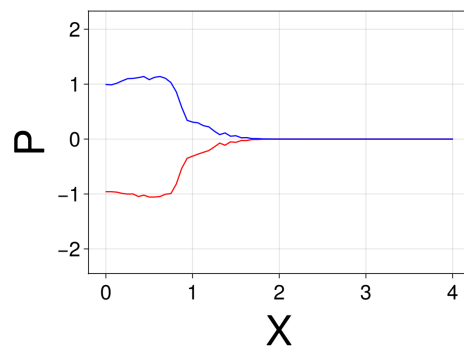


(f) $\sigma = 1.0$

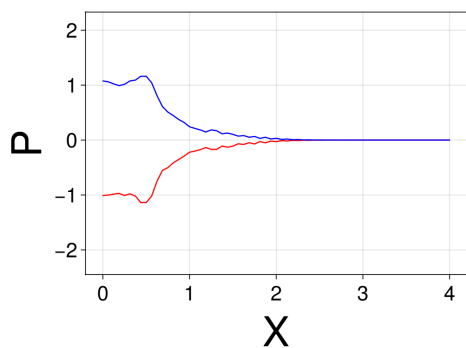
Figure 5.4: Pressure vs τ



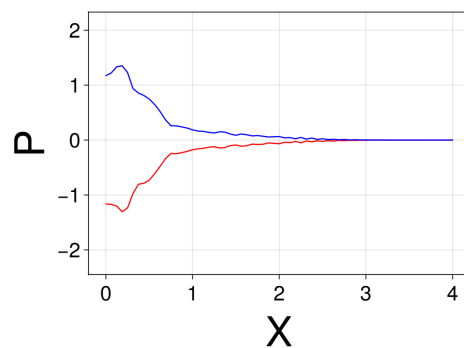
(a) $\sigma = 0.0$



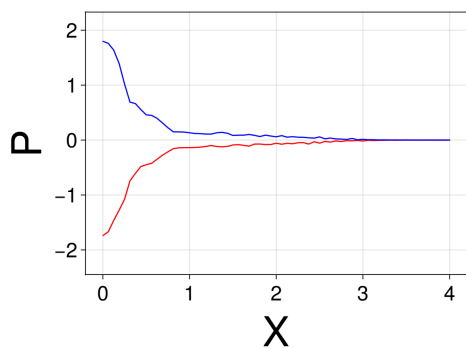
(b) $\sigma = 0.2$



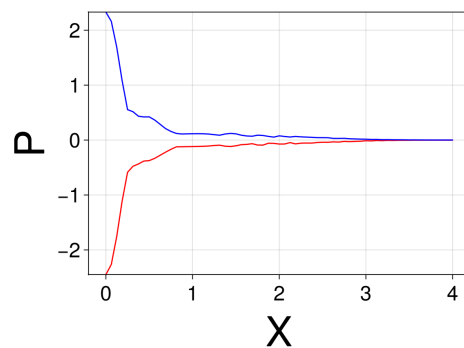
(c) $\sigma = 0.4$



(d) $\sigma = 0.6$



(e) $\sigma = 0.8$



(f) $\sigma = 1.0$

Figure 5.5: Pressure vs X

Chapter 6

Conclusion and Future Work

6.1 Conclusion

This thesis has focused on the development of a provably stable discretization of the KZK equations using a CG-SBP-SAT approach. The KZK equations, which model nonlinear wave phenomena such as absorption and diffraction, are particularly relevant for simulating the pressure propagation in HIFU applications.

To build up to the main results, the thesis begins by exploring the discretization of three foundational PDEs: the linear advection equation, the linear diffusion equation, and Burgers' equation. Each of these PDEs contains elements that are also present in the KZK equations. By performing a rigorous stability analysis on these simpler equations, the groundwork is laid for tackling the more complex KZK equations. These initial steps serve as a blueprint for the type of stability analysis needed for the KZK equation, guiding the construction of a stable discretization.

Central to this work is the use of SBP operators coupled with SATs to ensure stability. Chapter 3 introduces the concept of SBP operators, which are critical as they mimic the integration by parts principle, a fundamental tool in stability proofs for PDEs. The thesis demonstrates the construction of SBP operators within a CG framework and extends these local operators to global one-dimensional operators. These operators are then employed to discretize the linear advection, linear diffusion, and Burgers' equations, with SATs used to weakly enforce boundary conditions. The semi-discrete forms of these equations are proven to be stable, providing a solid foundation for the subsequent discretization of the KZK equations.

In Chapter 4, we present the primary contribution of this thesis: the discretization and stability analysis of the KZK equation. The analysis focuses on the dimensionless form of the KZK equation, which is essential for practical applications such as HIFU. The thesis extends the one-dimensional global CG operators to three dimensions using tensor products, proving that these extended operators satisfy the SBP property. These operators are applied to the KZK equation in a manner analogous to the linear PDEs discussed earlier. A key innovation in this chapter is the introduction of a modified second-derivative term, which is shown to be SBP. The construction of SATs for imposing Neumann and Dirichlet boundary conditions is also detailed, and the resulting semi-discrete form of the KZK equation is rigorously proven to be stable.

Chapter 5 evaluates the convergence, accuracy, and stability of the proposed discretization using the method of manufactured solutions. The thesis concludes by applying the developed scheme to a HIFU test case, inspired by prior research, thereby demonstrating the practical applicability of the discretization for simulating wave propagation in focused ultrasound.

6.2 Future work

While this thesis successfully develops a stable semi-discrete scheme for the KZK equation using the SBP-SAT technique on Cartesian meshes, there remain several avenues for future research and extension. One potential direction is to extend the current scheme to handle unfocused ultrasound. The dimensionless form of the KZK equation for unfocused ultrasound introduces additional complexities, such as terms involving $\frac{1}{4(1+\sigma)^2} \partial_\tau^{-1} \frac{\partial^2 \mathcal{P}}{\partial X^2}$ [45], which require careful consideration in the stability analysis. Another interesting extension would be to adapt the scheme to cylindrical coordinates, which are often used in HIFU applications. This adaptation would involve similar challenges to those encountered with unfocused ultrasound, particularly in the handling of additional terms and the construction of appropriate SBP operators.

Further, the current algorithm could be generalized to accommodate curvilinear coordinates, allowing for the modeling of wave propagation in more complex geometries. This would be particularly useful for simulating HIFU in anatomically accurate models, where Cartesian meshes may be insufficient.

Beyond the wave propagation modeling itself, future work could also explore coupling the current pressure-based model with a thermal model, such as the Bioheat equation. This would enable the simulation of tissue heating and provide a more comprehensive tool

for applications like cancer ablation, where understanding the temperature distribution is as critical as modeling the pressure waves.

By addressing these extensions, the work presented in this thesis could be significantly broadened, making it applicable to a wider range of ultrasound-based therapeutic and diagnostic applications.

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