Analysis of Boundary and Interface Closures for Finite Difference Methods for the Wave Equation

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Abstract

We consider high order finite difference methods for the wave equation in the second order form, where the finite difference operators satisfy the summation–by–parts principle. Boundary conditions and interface conditions are imposed weakly by the simultaneous–approximation–term method, and non–conforming grid interfaces are handled by an interface operator that is based on either interpolating directly between the grids or on projecting to piecewise continuous polynomials on an intermediate grid.

Stability and accuracy are two important aspects of a numerical method. For accuracy, we prove the convergence rate of the summation–by–parts finite difference schemes for the wave equation. Our approach is based on Laplace transforming the error equation in time, and analyzing the solution to the boundary system in the Laplace space. In contrast to first order equations, we have found that the determinant condition for the second order equation is less often satisfied for a stable numerical scheme. If the determinant condition is satisfied uniformly in the right half plane, two orders are recovered from the boundary truncation error; otherwise we perform a detailed analysis of the solution to the boundary system in the Laplace space to obtain an error estimate. Numerical experiments demonstrate that our analysis gives a sharp error estimate.

For stability, we study numerical treatments of non–conforming grid interfaces. In particular, we have explored two interface operators: the interpolation operators and projection operators applied to the wave equation. A norm–compatibility condition involving the interface operator and the norm related to the SBP operator is essential to prove stability by the energy method for first order equations. In the analysis, we have found that in contrast to first order equations, besides the norm–compatibility condition an extra condition must be imposed on the interface operators to prove stability by the energy method. Furthermore, accuracy and efficiency studies are carried out for the numerical schemes.
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List of Papers

This thesis is based on the following papers


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Chapter 1

Introduction

1.1 Scope

This thesis deals with numerical simulations of wave propagation problems, which has a wide range of scientific applications from transmission of sound in the air or ocean to seismic waves in the earth. Wave propagations are often modeled by time dependent linear partial differential equations. When a wave encounters an obstacle in the medium or travels across to another medium, certain phenomena could occur such as reflection or refraction, which are interpreted as boundary conditions and media interface conditions. It is a demanding task to develop accurate and efficient numerical methods to solve the governing equations. Furthermore, it is desirable to complement numerical methods by stability and accuracy analysis.

Among many numerical methods, high order finite difference methods are easy to programme and efficient when applied to solve wave propagation problems. Traditionally, a second order hyperbolic equation is written to a first order hyperbolic system, and is analyzed by the theories for such systems. This is mainly because both the theories and the numerical methods for first order hyperbolic systems have been largely developed. However, there are advantages [31] of analyzing and solving a second order hyperbolic equation directly in the second order form, which is thereby the focus of this thesis. The acoustic wave equation is chosen as the model equation because it is classical to investigate numerical methods for second order hyperbolic equations.

Two key points of a numerical method are stability and accuracy. A stable numerical scheme does not magnify approximation errors, while an unstable numerical scheme typically gives a numerical solution that deviates dramatically from the exact solution. For a stable finite difference method, the numerical solution converges to the true solution with a consistent ap-
proximation of the equation. The rate at which the numerical solution approaches the exact solution is referred to as the convergence rate, and is often used as the measure of accuracy. When solving an initial boundary value problem by a finite difference method, the large truncation error is typically localized near a boundary and interface, and its effect to the overall convergence rate has long been a research topic. In the pioneering work [19], it is shown that one order can be recovered from the localized truncation error for first order hyperbolic systems. The result is extended to parabolic problems in [61, 62]. Much work of this thesis is devoted to the proofs of the convergence rate for the summation–by–parts finite difference approximations of the wave equation with various boundary conditions and grid interface conditions.

The second focus of this thesis work is the numerical treatment of non–conforming grid interfaces in finite difference methods for the wave equation. In many applications, waves exhibit important features locally in a small subset of the domain. For an accurate and efficient numerical scheme, it is important that the mesh is only refined locally where necessary, and non–conforming grid interfaces are treated carefully to preserve the stability property and the high accuracy of the numerical scheme.

1.2 Outline

In Chapter 2, we introduce the governing equations of wave propagation problems, and the common numerical methods used to solve those equations. In particular, the summation–by–parts finite difference methods are discussed in detail. Chapter 3 focuses on the techniques of imposing boundary and grid interface conditions. In Chapter 4, we provide a summary and mention some future work.
Chapter 2

Background

2.1 Wave equation

The acoustic wave equation in one space dimension was first derived by d’Alembert in 1746 for the case of the vibrating string, and was suggested its applicability to model the propagation of sound in the air. In 1759, Euler derived the same equation based on the fluid dynamics principles, and shortly after that extended the equation to three space dimensions [58, 68]. For the derivation of the acoustic wave equation, we consider an ideal fluid described by its ambient state that is characterized by three ambient variables: pressure $p_0$, density $\rho_0$ and velocity $v_0$. These variables satisfy the corresponding fluid dynamics equations. A perturbation to the ambient state results in an acoustic disturbance and generates acoustic waves that propagate in the medium defined by the ambient state. The new ambient variables become $p = p_0 + u$, $\rho = \rho_0 + \rho'$ and $v = v_0 + v'$ where $u$, $\rho'$ and $v'$ represent the acoustic contributions. To describe acoustic waves, it is adequate to consider a quiescent medium that has zero velocity $v_0 = 0$ and time independent pressure and density, i.e. $\partial p_0/\partial t = \partial \rho_0/\partial t = 0$. The acoustic wave equation is then obtained by substituting the new ambient variables to the fluid dynamics equations and linearizing them [58]. The general form of the acoustic wave equation is

$$\frac{1}{c^2} u_{tt} = \rho_0 \nabla \cdot \left( \frac{1}{\rho_0} \nabla u \right), \quad (2.1)$$

where $u$ is the acoustic pressure and $c$ is the speed of acoustic wave propagation. In a homogeneous medium, the ambient variables are independent of the position, and Equation (2.1) is simplified to

$$u_{tt} = c^2 \Delta u. \quad (2.2)$$
The Laplacian operator is defined as the divergence of gradient, i.e. $\Delta u = \nabla \cdot \nabla u$. A function $F(x, t)$ can be added to the equation to model an external force.

An important second order system is the elastic wave equations that model the propagation of waves in elastic materials. There are two basic types of body waves in an elastic medium, namely the pressure wave and the shear wave. They travel with different wave speeds and can be transformed to each other upon encountering an interface, a phenomenon that is called mode conversion.

Both acoustic waves and elastic waves are mechanical waves, and they travel through a medium with an initial energy. The propagation of electromagnetic waves does not require a medium, and is modeled by the Maxwell’s equations, which can be either written as a second order partial differential equation or a first order hyperbolic system in terms of the electric field and the magnetic field.

The acoustic wave equation itself does not have a unique solution, and must be augmented with suitable initial conditions and boundary conditions. Due to the second order derivative in time, the initial data of $u$ and $u_t$ are needed. The problem is called Cauchy if the medium $\Omega$ spans the entire space. In this case, it is often for convenience assumed that the solution is periodic, and Fourier technique is used to solve the underlying equation. If the medium $\Omega$ has physical boundaries, suitable boundary conditions need to be provided in the model. This kind of problem is called an initial–boundary value problem. In reality, some waves propagate to a distance much longer than its wavelength, for example, the wave generated by an earthquake or a tsunami wave. To solve such a problem, we have to restrict to a smaller domain of interest, due to the limited computational resources. The challenge is to derive suitable artificial boundary conditions for the restricted domain so that the obtained solution converges to the solution of the original problem. Two common approaches are to use an absorbing boundary condition [14] or a perfectly matched layer [11]. Our focus in this thesis is the acoustic wave equation in a bounded domain with physical boundary conditions.

2.2 Well–posedness

Unlike the well–studied theories and numerical methods for first order hyperbolic systems, the current understanding of second order hyperbolic systems is limited. In fact, even for the continuous problem, the development is quite recent. In this section, we use the stability concepts introduced in [29] to analyze the continuous second order hyperbolic problems.
2.2. Well–posedness

The acoustic wave equation in two space dimensions is

\[ u_{tt} = u_{xx} + u_{yy} + F(x, y, t), \]
\[ u(x, y, 0) = f_1(x, y), \]
\[ u_t(x, y, 0) = f_2(x, y), \]

(2.3)

where \( x \geq 0, -\infty < y < \infty \) and \( t \geq 0 \). At the boundary \( x = 0, -\infty < y < \infty \), a boundary condition must be imposed. Two important types are the Dirichlet boundary condition

\[ u(0, y, t) = g(y, t), \]

(2.4)

and the Neumann boundary condition

\[ u_x(0, y, t) = g(y, t). \]

(2.5)

The forcing function \( F \), the initial data \( f_1, f_2 \) and the boundary data \( g \) are compatible smooth functions with compact support. With the variable \( x \) in a bounded domain, there is one boundary condition at each boundary. The problem in consideration here is half–line in \( x \), and the second boundary condition is replaced by requiring that the solution is bounded in \( L_2 \) norm for every fixed \( t \) : \( \| u \|^2 < \infty \) where the scalar product and norm are defined as

\[ (\omega_1, \omega_2) = \int_{-\infty}^{\infty} \int_0^{\infty} \omega_1 \omega_2 dx dy, \quad \| \omega_1 \|^2 = (\omega_1, \omega_1). \]

Equation (2.3) is well–posed if there exists a unique solution that depends continuously on the data. To show existence of a solution, we Laplace transform in \( t \) and Fourier transform in \( y \) of Equation (2.3), which yields a linear second order ordinary differential equation in \( x \). With the boundary condition (2.4) or (2.5) and the condition \( \| u \|^2 < \infty \), a solution in Fourier and Laplace space is obtained. The corresponding solution in the physical space is obtained by an inverse Fourier and Laplace transform.

A common way to show that the solution depends continuously on the data is to derive an estimate of the solution in terms of the data in some norm, which then guarantees that a small perturbation in the data causes only a small perturbation in the solution for a linear problem. For a first order hyperbolic system, the estimate of the solution is often obtained through the energy method, and the estimate is referred to as the energy estimate. It is shown in [29] that for a second order hyperbolic system, we need a standard energy estimate and boundary stability to make sure that the solution depends continuously on the data. Boundary stability [29, Definition 2.3] is defined as: Equation (2.3) is boundary stable if with \( F = 0 \) and \( f_1 = f_2 = 0 \).
there are constants $\eta_0 \geq 0$, $K > 0$ and $\alpha > 0$, which are independent of $g$, such that for all $\eta > \eta_0$, $T \geq 0$,

$$\int_{0}^{T} e^{-2nt} \int_{-\infty}^{\infty} |u(0, y, t)|^2 dy dt \leq \frac{K}{\eta^\alpha} \int_{0}^{T} e^{-2nt} \int_{-\infty}^{\infty} |g(y, t)|^2 dy dt.$$

Clearly, Equation (2.3) is boundary stable with the Dirichlet boundary condition. It is more involved to show boundary stability with the Neumann boundary condition. We refer to [29, Theorem 3.8] for a detailed proof by the Laplace transform technique.

To derive a standard energy estimate, we multiply Equation (2.3) by $u_t$ and use the integration–by–parts rule in $x$ and $y$, and obtain

$$\frac{d}{dt} (\|u_t\|^2 + \|u_x\|^2 + \|u_y\|^2) = 2 \int_{-\infty}^{\infty} \int_{0}^{\infty} u_t F \, dx \, dy$$

(2.6)

with either the homogeneous Dirichlet or Neumann boundary condition.

Define the continuous energy $E = \|u_t\|^2 + \|u_x\|^2 + \|u_y\|^2$, it follows

$$\sqrt{E} \leq \sqrt{\| (f_1)_x \|^2 + \| (f_1)_y \|^2 + \| f_2 \|^2} + \int_{0}^{t} \| F(\cdot, \cdot, z) \| dz.$$  

(2.7)

The uniqueness of the solution follows from the existence of the solution and the energy estimate. Consequently, Equation (2.3) is well–posed.

The motivation of the stability concepts in [29] is that they are robust in the sense that a small perturbation in the data or the equation does not destroy the well–posedness. The robustness also allows us to localize the problem, i.e. to decompose a general initial boundary value problem to a Cauchy problem and initial boundary value problems in half spaces. If all the decomposed problems are well–posed, the original problem is also well–posed.

In contrast to first order hyperbolic equations for which the energy is often the norm of the solution, here the continuous energy $E$ is a semi–norm as the solution $u$ itself is not included. By using the following relation

$$\frac{d}{dt} \|u\|^2 = (u, u_t) + (u_t, u) \leq \|u\|^2 + \|u_t\|^2,$$

we can include $u$ in a new energy $\tilde{E} = \|u\|^2 + \|u_t\|^2 + \|u_x\|^2 + \|u_y\|^2$ and derive an energy estimate for $\tilde{E}$ with the estimate including a growth in time. It is more convenient to use the energy $E$ in the stability analysis, and a discrete analog of $\tilde{E}$ in the convergence verification.

In [29], it is shown that Equation (2.3) with the boundary condition

$$u_x = ibu_y + g, \ b \text{ real, } 0 < |b| < 1$$


2.3. Numerical methods

is also well-posed. In this case, Equation (2.3) admits the solution

\[ u = e^{-|b\omega|x}e^{i\omega(y\pm\sqrt{1-b^2}t)}, \quad (2.8) \]

which decays exponentially in \( x \) and oscillates in \( y \). The solution (2.8) represents a surface wave, and is also supported by the elastic wave equations with the traction free boundary condition.

2.3 Numerical methods

With a special setting of the domain geometry and the medium property, the analytical solution of the wave equation could be obtained by the method of separation of variables. In a realistic problem with a complex geometry and a heterogeneous medium, analytical method is often not feasible. Numerical simulation is an alternative and a strong tool to solve more difficult problems in applications. It has been demonstrated that high order accurate time stepping methods as well as high order accurate spatial discretizations are more efficient to solve wave propagation problems on smooth domains [20, 23, 28]. High order methods use less number of grid points per wavelength at least if the accepted error level is low enough.

There are essentially two phases in the numerical integration of time dependent partial differential equations: the approximation of spatial derivatives and temporal derivatives. We consider the method of line approach, that is to first approximate the spatial derivatives only and leave the time variable continuous. This results in a semi-discretized system of ordinary differential equations, which is then solved by a suitable time integrator. In this section, we first discuss the most commonly used numerical methods for the approximation of spatial derivatives in wave propagation problems, with an emphasis on high order accurate finite difference methods, and then remark on some time integrators suitable for the resulting system of ordinary differential equations.

One of the simplest and oldest numerical methods for the numerical solution of partial differential equations is finite difference method. Traditionally, the acoustic wave equation is rewritten to a first order hyperbolic system, and then solved by the appropriate finite difference schemes. This is in part due to the well developed theories and numerical methods for first order hyperbolic systems [20, 21, 22, 27]. However, this approach has some drawbacks. Consider Equation (2.3) with zero forcing, and let \( z = [u_x, u_y, u_t]^T \). The corresponding first order hyperbolic system is

\[ z_t = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} z_x + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} z_y. \quad (2.9) \]
The number of unknowns in the semi–discretized equation is tripled, which leads to more computational work. Moreover, by solving (2.9) we only get an approximation of $u_t$, $u_x$ and $u_y$. An additional time integrator is needed to obtain the approximation of the unknown $u$. Therefore, it is preferable to solve the acoustic wave equation directly in the second order form, without rewriting it to a first order system.

In the finite difference framework, the computational domain is discretized into uniform intervals in each spatial coordinate to construct a grid. The derivative at each grid point is approximated by using the function values at nearby grid points with a set of weights [15]. Central finite difference schemes can be used in the interior of the computational domain, while near the boundaries special boundary stencils are needed. From the accuracy point of view, it is desirable to use a boundary stencil that is as accurate as the interior stencil. However, in many cases the boundary stencil has an accuracy reduction due to stability reasons. One such example is the summation–by–parts (SBP) finite difference operators that will be discussed in Section 2.4.

With a $2p^{th}$ order accurate standard central finite difference scheme for the approximation of first and second derivative, the bandwidth of the stencil is $2p + 1$. From the computational point of view, it is desirable to use a scheme with a minimum bandwidth. Compact finite difference schemes (Padé type approximations) have smaller bandwidths and also smaller leading error coefficients than the standard central finite difference schemes for the same order of accuracy. The drawback is that a tridiagonal or pentadiagonal system has to be solved in each time step. They are introduced in [10] and discussed in [20]. In [7], a compact finite difference scheme with fourth order accuracy in time and space is developed for the acoustic wave equation.

Finite difference method in its basic form is restricted to handle rectangular shaped domains. When a complex geometry is present, one approach is to partition the computational domain into blocks and use a curvilinear grid in each block to resolve the boundary feature. In this case, suitable interface conditions have to be imposed on the interfaces between adjacent blocks. This leads to the difficulties of numerical interface treatments, which should guarantee stability and preserve high accuracy of the numerical scheme. Moreover, the resulting transformed equation has second derivative terms with variable coefficients and mixed–derivative terms even if the original equation has only constant coefficients. In [65], a high order SBP finite difference scheme is developed to solve the acoustic wave equation in three space dimensions in a domain with a complex geometry and a heterogeneous medium. The complex geometry is resolved by curvilinear grid, and the computational domain is divided into blocks where the medium dens-
ity is smoothly varied in each block and the grid interfaces are conforming. The blocks are patched together by the simultaneous-approximation-term (SAT) technique.

With a very complex geometry, it is not obvious how to partition the computational domain and construct a curvilinear grid of high quality. In this case, an alternative is to use a standard Cartesian grid without requiring the boundaries to be aligned with the axes, which is often called embedded boundaries or immersed boundaries. Embedded boundary conditions for the acoustic wave equation have been discussed in several papers. In [1] a second order accurate scheme is developed where the Dirichlet boundary condition is imposed weakly by the SAT method. Though the analysis of the problem in one space dimension shows the truncation error $O(h^2)$, the numerical solution of a problem in two space dimensions converges cubically. In [31], a provably stable second order accurate scheme is constructed for the problem in two space dimensions with the Dirichlet boundary condition, which is imposed by using exterior ghost points. The scheme is further extended to solve the problem with the Neumann boundary condition in [32], and a small dissipative term is added to stabilize the scheme. Recently, a fourth order accurate Padé type discretization is developed in [5]. The boundary condition is imposed by using interior ghost points, and instability is overcome by adding artificial dissipations. Rigorous stability and accuracy analysis seem very difficult for the high order accurate finite difference schemes applied to problems with embedded boundaries.

Another important numerical technique to solve partial differential equations is the finite element method [36]. The computational domain is divided into structured or unstructured cells, for example, triangles or quadrilaterals in two space dimensions and tetrahedrons or hexahedrons in three space dimensions. With an unstructured grid, a complex geometry can be represented in a straightforward and accurate manner. A finite element method starts with rewriting the differential equation to a weak formulation by multiplying the equation by a test function in some appropriate function space $V$ and integrating in space. Neumann boundary condition is usually imposed weakly, but Dirichlet boundary condition is imposed strongly. Next, the finite element discretization is obtained by restricting the test function to a much smaller subspace $V_h$ of $V$, and fixing the solution on the Dirichlet boundary by the Dirichlet boundary condition. The space $V_h$ often consists of continuous piecewise polynomials on the grid, and the order of the polynomials determines the convergence rate of the numerical scheme. It is also possible to impose the boundary conditions weakly by the Nitsche’s method [25].

Although the finite element method is flexible with boundary configurations, there are certain disadvantages of this method. An unstructured grid
often leads to less regular matrices in discretization and it is more difficult to program in a computationally efficient way. The construction of a high quality mesh is a non–trivial task in three space dimensions. Moreover, the mass matrix arising from the spatial discretization must be inverted in each time step. The mass–lumping technique can be used to make the mass matrix diagonal, but introduces instabilities for high order accurate schemes on triangular meshes. The instability issue is overcome in [9] by using special quadrature rules. A special form of finite element method is obtained by using Lagrange polynomials with Gauss–Lobatto–Legendre collocation points as the trial functions, and is referred to as spectral element method with the attractive features of high accuracy and a diagonal mass matrix.

The discontinuous Galerkin method, which allows discontinuities of the solution and the test functions at the nodes, is another type of finite element method. It is originally developed to solve first order equations, and is also successfully used to solve the second order wave equation [18]. The discontinuous Galerkin method is flexible in handling complex geometries and hanging nodes, but requires a small time step due to the stiffness. The relation between the SBP–SAT finite difference method and the discontinuous Galerkin spectral element method is explored in [16].

Finite volume method is a conservative method and can be used on a structured or unstructured mesh. It is ideal for conservation law problems, and is used in many computational fluid dynamics packages. For example, finite volume method is implemented in the software Clawpack to solve the acoustic wave equation in the first order system form [37].

After the approximation of spatial derivatives in the method of line approach, we get a large system of second order ordinary differential equations of the type

$$v_{tt} = Qv + F. \quad (2.10)$$

With an explicit time stepping method, the expected stability condition is $$\Delta t \leq Ch/\sqrt{d}$$ where $$d$$ is the space dimension and $$C$$ is a constant independent of $$h$$ [49]. This is in many cases not a severe constraint in the time step, and therefore explicit methods are often used to advance (2.10) in time. For example, the classical Runge–Kutta method has the attractive feature of fourth order accuracy, and under certain conditions generalized stability is guaranteed if the semi–discretized equation is stable in the generalized sense [35]. However, it is only applicable to first order ordinary differential equations. We have to rewrite (2.10) to

$$\begin{pmatrix} v \\ v_t \end{pmatrix}_t = \begin{pmatrix} 0 & I \\ Q & 0 \end{pmatrix} \begin{pmatrix} v \\ v_t \end{pmatrix} + \begin{pmatrix} 0 \\ F \end{pmatrix},$$

which doubles the number of unknowns. To solve the second order system (2.10) directly, the modified equation approach can be used. The idea is to
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start with the second order accurate approximation of \( v_{tt} \) and replace higher order derivatives in the truncation error by the equation itself. In this way, high order accuracy is achieved for the approximation of \( v_{tt} \). Such schemes are developed in [17].

The well known SBP–SAT method for spatial discretizations is extended to the time domain in [38, 53] for first order initial value problems. The highlight is that it is high order accurate and unconditionally stable. Besides, a fully discrete energy estimate can be derived.

To advance the semi–discretized equation for the wave equation in time, the SBP–SAT technique for second order initial value problems is needed. This is discussed in [54], where it is found that the traditional compatible narrow SBP operators approximating second derivative cannot be incorporated since stability cannot be proved by the energy estimate. Instead, the SBP operators with wide stencils are used with a modified penalty term to impose weakly the initial conditions, and in this case an energy estimate is derived.

2.4 SBP operators

There are many kinds of finite difference methods that can be used to discretize a partial differential equation. For an equation with periodic boundary conditions, it is straightforward to achieve stability and high accuracy. In bounded domains, special stencils are used near the boundaries. If a numerical scheme is stable, the approximated solution is bounded by the data. With a consistent approximation of the derivatives, the error in the solution decays to zero as the mesh size tends to zero. Unstable numerical schemes are useless because a small perturbation, typically caused by round–off errors or fluctuations in the initial data, leads to an unrealistic growth in the numerical solution.

SBP operators are a particular kind of finite difference operators with standard central finite difference stencils in the interior and special boundary closures. Integration–by–parts is the key tool to prove well–posedness of the continuous problem by deriving an energy estimate. An SBP operator mimics integration–by–parts via its associated norm, and in many cases it is possible to derive a discrete energy estimate. The idea of SBP operators was originally discussed in [33, 34] in 1970s. Unfortunately, it was then somewhat forgotten for 20 years, probably due to the difficulties in the numerical boundary treatments. It has been developed constantly since 1990s after the introduction of suitable numerical boundary techniques. In the following, we discuss the SBP operators that are commonly used to approximate spatial derivatives.
Let the unit interval $[0,1]$ be discretized by a uniform grid

$$x_j = jh, \quad j = 0, \ldots, n,$$

where $h$ is the mesh size. Let $u(x)$ be a smooth function in $[0,1]$ and $v = [v_0, \ldots, v_n]^T$ be the projection of $u(x)$ on the grid: $v_j = u(x_j)$. $D_1$ is a diagonal norm SBP operator approximating first derivative if

$$D_1 = H^{-1}Q, \quad Q + Q^T = B = \text{diag}(-1,0\cdots,0,1),$$

where $H$ is diagonal positive definite with interior elements $h$ and special elements near the boundary. $H$ defines the norm associated with the SBP operator. The accuracy of the SBP operator is often termed as $2p^{th}$ order accuracy, which means that the approximation error is $O(h^{2p})$ in the interior, but increases to $O(h^p)$ near the boundary. That is,

$$(D_1 v)_j = \begin{cases} u_x(x_j) + O(h^{2p}) & \text{if } j = n_p, \cdots, n - n_p, \\ u_x(x_j) + O(h^p) & \text{otherwise} \end{cases}$$

where $n_p$ is the number of grid points with special boundary stencils, and $n_p$ depends on $p$ but not $h$.

Up to $8^{th}$ order SBP operators $D_1$ are constructed in [60], where the values of $n_p$ are $n_p = 1, 4, 6, 8$ for $p = 1, 2, 3, 4$. The accuracy is further increased to $10^{th}$ order with $n_p = 11$ in [41]. One may initially expect to use 10 grid points for the boundary closure of the $10^{th}$ order accurate $D_1$, but it turns out that such an operator cannot be constructed; therefore 11 boundary points are used. This motivates a recent work in [2], where an algorithm is developed to determine the minimum value of $n_p$ for a given $p$. The result shows that $n_p$ increases quickly with respect to the increment of $p$, for example $n_p = 71$ when $p = 15$. It’s in doubt if these very high order accurate SBP operators have any usefulness in practice since they require a large number of boundary points. Nevertheless, $12^{th}$ and $14^{th}$ order accurate SBP operators $D_1$ are constructed in [2] with 14 and 19 boundary points, respectively.

To solve problems involving second derivative terms in space like the acoustic wave equation and the elastic wave equations, an SBP operator $(D_2 v)_j \approx u_{xx}(x_j)$ is needed. Such operators based on diagonal norms are constructed in [46] up to $8^{th}$ order accuracy and in [41] for $10^{th}$ order accuracy in the form

$$D_2 = H^{-1}(-M + BS),$$

where $H$ is the diagonal norm, $M$ is symmetric positive semidefinite and $B = \text{diag}(-1,0,\cdots,0,1)$. The first and last row of $S$ approximate first
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derivative at the boundaries with an approximation error $O(h^{p+1})$. The SBP operator $D_2$ has a similar accuracy property as $D_1$:

$$(D_2v)_j = \begin{cases} 
  u_{xx}(x_j) + O(h^{2p}) & \text{if } j = n_p, \ldots, n - n_p, \\
  u_{xx}(x_j) + O(h^p) & \text{otherwise} 
\end{cases}$$

It is important that $D_1$ and $D_2$ are based on the same norm so that the energy method is applicable to prove stability for problems with both first derivative and second derivative terms, for example the convection–diffusion equation.

Another way to approximate second derivative is to use $D_1$ twice yielding $(D_1 D_1 v)_j \approx u_{xx}(x_j)$. However, this approach has two drawbacks. Firstly, for the same interior accuracy order the resulting operator $D_1 D_1$ has a wider stencil and a larger approximation error than $D_2$, which lead to more computational work and larger error in the numerical solution. This motivates the definition narrow in [48], which means that the interior stencil width of the SBP operator is minimum. Secondly, the highest frequency mode $[1, -1, \ldots, -1, 1]^T$ that can exist on the grid is in the null space of $D_1$ and $D_1 D_1$, and cannot be damped out. As a consequence, spurious oscillations occur in the nonlinear regime for nonlinear equations [63].

In [48], an important relation between $D_2$ and $D_1$, namely compatibility, is introduced. If $D_1$ and $D_2$ are compatible, $D_2$ is essentially $D_1 D_1$ plus a small dissipative term:

$$D_2 = H^{-1}(-D_1^T H D_1 - R + BS), \tag{2.12}$$

where the remainder $R$ is symmetric positive semidefinite. Compatibility is important in the stability proof of the SBP–SAT method applied to problems with a combination of mixed ($\partial^2 / \partial x \partial y$) and non–mixed ($\partial^2 / \partial x^2, \partial^2 / \partial y^2$) second derivative terms, for example the elastic wave equations and compressible Navier Stokes equations. The SBP operators $D_1$ and $D_2$ in [46] are compatible up to $8^{th}$ order accurate, but the $10^{th}$ order accurate SBP operators $D_1$ and $D_2$ in [41] are not compatible.

In real–world applications, the acoustic wave often propagates in a medium with a complex geometry, which can be resolved by using a curvilinear grid. As a consequence, terms with variable coefficients $(b(x) u_x)_x$ appear in the transformed equation even if the original equation has constant coefficients. Hence, there is the need of the SBP operator approximating the second derivative with a variable coefficient $(D_2^{(b)} v)_j \approx (b u_x)_x|_{x=x_j}$ where $b = b(x) > 0$ is a known function.

In [39], narrow diagonal norm SBP operators $D_2^{(b)}$ are constructed up to $6^{th}$ order accuracy. The construction is based on an ansatz derived from
(2.12) with the unknowns in the boundary closure of the corresponding remainder term. This results in a large system of nonlinear equations, which is different from the cases of constructing $D_1$ and $D_2$ where only linear equations need to be solved. These operators $D_2^{(b)}$ are compatible with the operators $D_1$ constructed in [60].

It is possible to improve the accuracy of the first and second derivative SBP operators so that the approximation error is $O(h^{2p})$ in the interior and $O(h^{2p-1})$ near the boundaries. In this case, the norm $H$ is no longer diagonal. Instead, it has a block structure near the boundaries, and is referred to as a full norm or block norm. SBP operators approximating first derivative and second derivative with constant coefficients based on full norms are constructed in [41, 46, 60]. Though they have a better accuracy property, they are not widely used in practice due to instability issues for the wave equations with variable coefficients, or problems solved on a curvilinear grid. In [41], boundary dissipation terms are introduced to stabilize the scheme. Stability is verified by eigenvalue analysis and demonstrated in the numerical experiments. SBP operators approximating second derivatives with variable coefficients based on full norms have not yet been constructed. The numerical experiments in [41] indicate that there is little need to do so since there is no accuracy reduction by applying the full norm SBP operator $D_1$ twice to approximate the second derivative.

Another way of improving accuracy is to allow non-equidistant grid near the boundary [42]. In this case, an optimization problem is solved to minimize the coefficient of the leading order approximation error near the boundary. Even though the theoretical approximation error near the boundary is still $O(h^p)$, numerical experiments demonstrate that these newly developed SBP operators are much more accurate with a practical value of $h$.

It is straightforward to extend the SBP operators to more than one space dimensions by using Kronecker products. If $U$ is an $m \times n$ matrix and $V$ is a $p \times q$ matrix, the Kronecker product $U \otimes V$ is the $mp \times nq$ matrix

$$U \otimes V = \begin{bmatrix} u_{11}V & \cdots & u_{1n}V \\ \vdots & \ddots & \vdots \\ u_{m1}V & \cdots & u_{mn}V \end{bmatrix}.$$ 

The SBP operators in two space dimensions $D_{xx}$, $D_{yy}$ are obtained through the corresponding SBP operators in one space dimension

$$D_{xx} = D_{xx} \otimes I_y, \quad D_{yy} = I_x \otimes D_{yy},$$

where $I_x$ and $I_y$ are identity matrices.

In the end, we mention that diagonal norm SBP operators approximating third and fourth derivatives are constructed in [40] for up to sixth order
2.4. SBP operators

accuracy. These SBP operators are based on different norms $H_{new}$ from the previously constructed first and second derivative SBP operators. Fortunately, new SBP operators based on $H_{new}$ approximating first and second derivatives are also constructed in [40] to ensure a practical usefulness.
Chapter 3

Boundary and grid interface treatment for finite difference methods

A main difficulty of using finite difference methods to solve an initial–boundary value problem is the numerical treatment of boundary conditions and grid interface conditions. An SBP operator itself does not impose any boundary conditions, and suitable techniques must be employed for its numerical treatment. Two main approaches are to impose boundary condition strongly and impose boundary condition weakly.

One way to impose the boundary condition strongly is to use the injection method by fixing the solution at the boundary with the boundary data for the Dirichlet boundary condition, and using exterior ghost points for the Neumann boundary condition. The injection method is easy to use but often leads to instabilities for high order accurate method, and is only used in special cases. An alternative of the strong enforcement of boundary conditions is to use the projection method [55, 56], where the Dirichlet and Neumann boundary conditions are imposed by a projection operator. Together with the SBP finite difference approximation of derivatives, stability can be guaranteed by deriving a discrete energy estimate, but in more than one space dimension there are difficulties in the corners of the computational domain.

In contrast, the weak enforcement of boundary conditions by the SAT method has gained great popularity because it is straightforward to understand and easy to program. Moreover, in many cases it is possible to derive a discrete energy estimate when the SAT method is used together with the finite difference operators satisfying the SBP properties. These techniques are discussed in more detail in Section 3.1.
Grid interfaces are created by partitioning the computational domain into blocks, and the blocks could either be conforming or non–conforming. As an example, the square–shaped computational domain is partitioned into four blocks shown in Figure 3.1. The partitioning in Figure 3.1a results in conforming blocks since the corners meet with each other, whereas in Figure 3.1b they are non–conforming blocks, and the interfaces are called T–junction interfaces. In each block, a grid is then generated, and if on a grid interface the grid points in the two adjacent blocks coincide, the grid interface is said to be conforming; otherwise it is a non–conforming grid interface.

In [65], a high order accurate finite difference method is developed to solve the acoustic wave equation on a mesh with conforming blocks and conforming grid interfaces. For the other mesh configurations, certain interpolations are needed for the communication of the data in adjacent blocks. The interpolations must preserve the stability property of the numerical scheme, and ideally also its convergence rate. In Section 3.2 we discuss two techniques to handle non–conforming blocks and grid interfaces, the interpolation operators [43] and the projection operators [26]. The interpolation operators handle conforming blocks with non–conforming grid interfaces for some grid refinement ratios, and the projection operators are more powerful since they can treat non–conforming blocks with non–conforming grid interfaces. The accuracy of these techniques is further discussed in Section 3.3.

There are also other methods for the numerical treatment of grid interfaces. One approach is to use ghost points near the grid interface as shown in Figure 3.2a with ghost points denoted by circles. In [50, 57], a second order accurate numerical scheme is developed to solve the elastic wave equation in the second order form, where the non–conforming grid interface is handled by introducing ghost points, and the scheme is implemented in the software
package WPP (Wave Propagation Program). The scheme is extended to fourth order accurate in [59] and is implemented in the software package SW4 (Seismic Waves, 4th order) [64].

With a very complex geometry, it is not easy to partition the computational domain in a good manner. An alternative is to allow two adjacent blocks to overlap, resulting in an overlapping grid depicted in Figure 3.2b. Overture [24] is a software package that simulates wave propagation problems and flow problems in complex moving geometries by using overlapping grids. One of the programs in Overture solves the elastic wave equation on an overlapping grid with different constitute parameters and domain geometries in both two and three space dimensions [3].

3.1 Boundary condition

3.1.1 Strong enforcement

To impose boundary conditions strongly, one way is to modify the SBP operators so that the boundary condition is embedded by the injection method. The boundary condition is fully satisfied without errors. However, the resulting difference operators usually do not satisfy the SBP properties anymore. Therefore, it is in many cases impossible to obtain a discrete energy estimate. Even for the simple scalar advection equation, the simulation with the sixth order accurate block norm SBP operator and injection method blows up quickly, indicating that the scheme is unstable [6]. An exceptional case is to use the diagonal norm SBP operators with the injection method to solve the wave equation with Dirichlet boundary conditions, for which the stability of the numerical scheme is proved in [12].

Another technique to impose the boundary condition strongly is the pro-

(a) A grid with ghost points (b) An overlapping grid

Figure 3.2: Non–conforming grid interfaces
projection method. The idea is to impose the boundary conditions by an orthogonal projection operator and together with the SBP property, a discrete energy estimate is obtained to ensure stability. The projection technique is developed in [55, 56] for first order hyperbolic, parabolic and mixed–hyperbolic–parabolic systems. Later, in [47] the technique is used for the numerical treatment of boundary conditions for the acoustic wave equation in the second order form. It has also been used for the numerical treatment of interface conditions when a piecewise continuous medium is present in the model. The drawback of the projection method is that it is often very difficult to use in practice. In more than one space dimension, when a corner is present due to the intersection of boundaries or grid interfaces, only one boundary condition is allowed at each corner point. Therefore, special treatment has to be taken to the corner points.

In Lawrence Livermore National Laboratory, the Serpentine project develops finite difference methods to solve wave propagation problems. There the boundary condition is enforced by using exterior ghost points. A boundary modified fourth order accurate approximation of the second derivative with a variable coefficient is developed in [59]. The approximation satisfies the SBP property, but is different from the SBP operators constructed in [39]. Stability is proved by the energy method and fourth order accuracy is verified in numerical experiments. Another ghost point approach is proposed in [23], where one or two interior ghost points are used to enforce the boundary conditions. The highlight is that very high accuracy (up to 12th order) can be achieved in the interior and the boundary closure is of the same accuracy. However, it lacks an energy estimate to guarantee stability. Instead, the stability analysis is carried out numerically by the Laplace transform technique.

### 3.1.2 Weak enforcement

A weak enforcement of a boundary condition via an SAT, often referred to as a penalty term, is introduced in [6]. Together with the SBP operators, the penalty parameters are chosen so that a discrete energy estimate is obtained. This methodology is often called the SBP–SAT finite difference method. It is straightforward to understand, easy to programme, and avoids the difficulties of the projection method on the corner points. In the following, we use the acoustic wave equation (2.3) with the homogeneous Neumann condition to demonstrate how to obtain a stable scheme in the SBP–SAT framework. The semi–discretized equation is

\[ v_{tt} = D_{xx} v + D_{yy} v + F + SAT_N \]  

(3.1)
where \( v \) is the discrete solution vector and \( SAT_N \) is the penalty term that imposes weakly the homogeneous Neumann boundary condition

\[
SAT_N = \tau_N H^{-1}(E_{0x} S_x v - 0),
\]

(3.2)

where \( E_{0x} \) picks up the numerical solution on the boundary points and \( \tau_N \) is the penalty parameter to be determined by the energy method so that an energy estimate exists. We multiply (3.1) by \( v^T_t H \), and obtain

\[
v^T_t H v_{tt} = v^T_t (-M_x - E_{0x} S_x) v + v^T_t (-M_y) v + v^T_t HF + \tau_N v^T_t E_{0x} S_x v.
\]

By choosing \( \tau_N = 1 \), we obtain

\[
v^T_t H v_{tt} = v^T_t (-M_x) v + v^T_t (-M_y) v + v^T_t HF.
\]

Taking the transpose of the above equation and adding it to itself yields

\[
\frac{d}{dt} \left( \|v_t\|^2_H + \|v\|^2_{M_x} + \|v\|^2_{M_y} \right) = 2v^T_t HF.
\]

(3.3)

Equation (3.3) is the discrete analogue of (2.6) with the corresponding discrete energy \( E_d(t) = \|v_t\|^2_H + \|v\|^2_{M_x} + \|v\|^2_{M_y} \). We then integrate (3.3) in time to get the discrete energy estimate

\[
\sqrt{E_d(t)} = \sqrt{E_d(0)} + \int_0^t \|F(z)\|_H dz,
\]

and the discretization is stable.

It seems difficult to impose the Dirichlet boundary condition for the acoustic wave equation in the second order form by the SAT method. The difficulty is overcome in [4], and the numerical scheme, which yields a non–symmetric semi–discretized equation, is proved to be stable. In [45], a stable and symmetric semi–discretization is developed, where the penalty term for the homogeneous Dirichlet boundary condition is

\[
SAT_D = -H^{-1} S^T (E_{0x} v - 0) - \frac{\tau_D}{h} H^{-1}(E_{0x} v - 0).
\]

(3.4)

The penalty parameter \( \tau_D \) must be chosen large enough \( \tau_D \geq \tau_0 \) to ensure a discrete energy estimate. The value of \( \tau_0 \) depends on the order of accuracy of the SBP operator but not the mesh size \( h \), and is shown in [44, 45, 66]. A so–called borrowing trick is essential for the stability proof of the acoustic wave equation with the Dirichlet boundary conditions [44, 45, 66].
3.2 Grid interface condition

In a realistic acoustic problem, the medium often has a discontinuous density. To solve it numerically with high accuracy, one way is to divide the computational domain into blocks with a continuous medium density in each block. If the medium has a continuous density, it is typically not homogeneous and the wave speed varies in space. With a uniform mesh in the entire computational domain, the mesh size has to be small enough to resolve the region with the smallest wave speed. As a consequence, unnecessarily refined mesh is used elsewhere, which leads to a suboptimal performance of the numerical scheme. Therefore, it is often desirable to partition the domain into blocks and use appropriate mesh sizes in different blocks. Even in a homogeneous medium, we would like to use a refined mesh in the region where a complex geometry is present. This leads to the difficulties of handling non–conforming grid interfaces with hanging nodes, that is, the grid points in adjoining blocks do not match along the interface, for example the mesh in Figure 3.3a.

In this section, we discuss the commonly used techniques for the numerical treatment of grid interface conditions for the acoustic wave equation solved on the mesh in Figure 3.3a. Since the computational domain is partitioned into two blocks, it is more convenient to write the equation as

\[ u^{1}_{tt}(x,y,t) = u^{1}_{xx} + u^{1}_{yy} + F^{1}(x,y,t), \quad 0 \leq x \leq 1, \quad 0 \leq y \leq 0, \quad t \geq 0, \]

\[ u^{2}_{tt}(x,y,t) = u^{2}_{xx} + u^{2}_{yy} + F^{2}(x,y,t), \quad 0 \leq x \leq 1, \quad y \geq 0, \quad t \geq 0, \]

(3.5)

with an interface \( \Gamma \) located at \( 0 \leq x \leq 1, \quad y = 0 \), where \( u^{1} \) and \( u^{2} \) are solutions in the upper block and lower block, respectively. We use the same assumption of the initial and boundary data as for Equation (2.3), and focus on the interface condition for \( \Gamma \). Since the solution of the original equation is smooth by assumption, it is natural to require smoothness of the solution of (3.5) in the entire computational domain. The appropriate interface conditions are

\[ u^{1}(x,0,t) = u^{2}(x,0,t), \]

(3.6a)

\[ u^{1}_{y}(x,0,t) = u^{2}_{y}(x,0,t). \]

(3.6b)

Condition (3.6a) and (3.6b) impose the continuity of the solution and the continuity of the normal derivative of the solution across the grid interface, respectively.

3.2.1 Interpolation operators

In [43], the interpolation operators \( I_{F2C} \) and \( I_{C2F} \) are constructed, where the subscripts \( F2C \) and \( C2F \) refer to fine to coarse and coarse to fine, re-
3.2. Grid interface condition

![Grid Interface](image)

Figure 3.3: Non–conforming grid interfaces

spectively. The mesh blocks need to be conforming and the mesh refinement ratio is 1:2 as depicted in Figure 3.3a with the interface marked by the thick line. The technique can be used to construct interpolation operators for some other ratios (1:4,1:8,···). In the following, we describe the properties of the interpolation operators that will be used in the stability and accuracy analysis of the numerical schemes for the acoustic wave equation.

On the interface $\Gamma$, the grids in the upper block and lower block are denoted by

$$x_j = jh, \quad j = 0, \cdots, n,$$

$$\tilde{x}_j = j\tilde{h}, \quad j = 0, \cdots, m,$$  \hspace{1cm} (3.7)

with the corresponding numerical solutions

$$v^1 = [v^1_0, \cdots, v^1_n]^T \quad \text{and} \quad v^2 = [v^2_0, \cdots, v^2_m]^T.$$  \hspace{1cm} (3.8)

The equality $n = 2m - 1$ yields a 1:2 mesh refinement ratio. The key point in the SAT method is to use the difference of $v^1$ and $v^2$ as a penalty term in the numerical scheme. However, the vectors $v^1$ and $v^2$ are of different lengths due to the non–conforming grid interface. As a consequence, interpolations between grids are needed. The interpolation from the grid $x$ to $\tilde{x}$ can be expressed as: given $v^1$, which approximates the true smooth solution $u_\Gamma$ on the grid $x$, construct $\tilde{v}^1 = IF_{2C}v^1$ to approximate $u_\Gamma$ on the grid $\tilde{x}$. With $u^1_x$ and $u^1_{\tilde{x}}$ denoting the restriction of $u_\Gamma$ on the grid $x$ and $\tilde{x}$, the interpolation error can be written as $u^1_{\tilde{x}} - IF_{2C}u^1_x$. The interpolation from the grid $\tilde{x}$ to $x$ and the corresponding interpolation error can be stated in a similar way.

The interpolation operators in [43] are termed as $2p^{th}$ order accurate, which means that the interpolation error is $O(h^{2p})$ in the interior and is $O(h^p)$ near the edge of the interface, $p = 1, 2, 3, 4$. The $2p^{th}$ order accurate interpolation operators are used together with the $2p^{th}$ order accurate SBP operators, and the scheme is said to be $2p^{th}$ order accurate though the truncation error of the semi–discretized equation may not be $O(h^{2p})$ or
The number of grid points with the large interpolation error $O(h^p)$ only depends on $p$ and is not changed when the mesh is refinement.

The accuracy of the interpolation near the edge of the interface is reduced in order to satisfy the norm–compatibility condition

$$H_{1x}I_{C2F} = (H_{2x}I_{F2C})^T, \quad (3.9)$$

where $H_{1x}$ and $H_{2x}$ are the SBP norms in (2.11) in the $x$–direction of the upper and lower blocks, respectively. This condition is built–in as a constraint in the construction process, and is important because it makes the energy method applicable to prove stability for first order hyperbolic systems and the Schrödinger equation [52].

For the acoustic wave equation in the second order form, we have found in [67] that to employ the energy method, a second condition

$$K_1 := H_{1x}(I_{1x} - I_{C2F}I_{F2C}) \geq 0, \quad K_2 := H_{2x}(I_{2x} - I_{F2C}I_{C2F}) \geq 0, \quad (3.10)$$

must be satisfied. Here, $I_{1x}$ and $I_{2x}$ are identity matrices, and the notation $K_{1,2} \geq 0$ means that $K_{1,2}$ is symmetric positive semidefinite. The eigenvalue analysis of (3.10) in [67] shows that (3.10) is satisfied for the second and fourth order accurate cases, and stability of the numerical scheme is proved by the energy method. No energy estimate can be derived for the sixth and eighth order accurate scheme. We have observed in the numerical experiment that the sixth order accurate scheme is stable when solving the acoustic wave equation on a Cartesian grid, but not on a curvilinear grid, and the eighth order accurate scheme produces a solution that blows up quickly on both grids.

In [67], we have also found that the convergence rate is lowered by one order by using the interpolation operators constructed in [43], compared with the case with a conforming grid interface. Nevertheless, an efficiency study demonstrates that in certain cases it is beneficial to use non–conforming grid interfaces, albeit the accuracy reduction.

The interpolation operators can be used to handle the grid interfaces in a multiblock mesh depicted in Figure 3.3b with the grid interfaces marked by thick lines. For stability reason, the dashed line must be considered as a grid interface so that non–conforming blocks are avoided. Since the accuracy of derivative approximations is lower near the grid interface, it is desirable to use as few grid interfaces as possible. If we do not consider the dashed line as a grid interface, then a T–junction interface is present in the mesh. As a consequence, in the left domain the SBP norm has the interior weight at the grid points near the T–junction intersection, while the SBP norms on the two right domains both have the boundary weights. This causes instabilities for higher order accurate schemes with $p \geq 2$ because the
norm–compatibility condition is violated. In [51], the T–junction operators are constructed for $p = 2, 3$ and 4 to overcome the instability problem and are applied to the advection equation and the Schrödinger equation.

### 3.2.2 Projection operators

A new methodology for the numerical treatment of grid interface conditions by projection operators is developed in [26], which handles non–conforming grid interfaces in a mesh with non–conforming blocks without a strict requirement on the mesh refinement ratio. We illustrate its basic idea in the flowchart shown in Figure 3.4, where the grids $x_j$ and $\tilde{x}_j$ in (3.7), and the numerical solutions $v^1$ and $v^2$ in (3.8) are used. The finite difference solutions $v^1, v^2$ are projected to subspaces $Q^1, Q^2$ of piecewise continuous polynomials corresponding to the grids $x_j, \tilde{x}_j$, and then projected to $Q$, a subspace of piecewise continuous polynomials corresponding to the union of the grids $x_j$ and $\tilde{x}_j$. Once the discrete finite difference solutions are projected to the same space $Q$, it is straightforward to construct the penalty term SAT$_Q$ there. The penalty term is then projected back to SAT$_1$ and SAT$_2$ on the grids $x_j$ and $\tilde{x}_j$. The key point of this new methodology is that the penalty terms are derived in a common space to which the finite difference solutions are projected. It seems that it involves more conceptual difficulties, but it
is a more flexible technique in several ways:

1. It handles non–conforming grid interfaces including T–junction cases in a straightforward manner. In addition, there is no strict requirement of the mesh refinement ratio in the adjacent blocks.

2. Besides the coupling of finite difference methods, it can also couple a finite difference method and an unstructured triangle–based discontinuous Galerkin method.

3. Up to 10\textsuperscript{th} order accurate projection operators are constructed. In the interior the projection error is $O(h^{2p})$ while near the edge the projection error is $O(h^p)$, $p = 1, 2, 3, 4, 5$. Similar to the interpolation operators, the number of grid points with the large projection error $O(h^p)$ is finite and is independent of $h$.

In [67], we use the projection operators along with the SBP–SAT method to solve the acoustic wave equation in the second order form. The connection between interpolation operators and projection operators is discussed, and the comparison between these two techniques is carried out in numerical experiments. To derive an energy estimate for stability, an analog of condition (3.9) and (3.10) must be satisfied. Similar to the interpolation operators, condition (3.9) is satisfied for all projection operators since it is a constraint in the construction process of the projection operators, but condition (3.10) is only satisfied for the second and fourth order accurate projection operators. However, in all the numerical experiments conducted in [67], the numerical scheme is stable for all projection operators up to tenth order accuracy.

We remark that the newly developed projection operators in [26] are altogether irrelevant to the projection operators in [55, 56] that are used to strongly impose boundary and interface conditions.

### 3.3 Accuracy

The truncation error in the semi–discretized equation is caused by the approximation of spatial derivatives. When using the SBP–SAT method to solve the acoustic wave equation in one space dimension, the truncation error is $O(h^{2p})$ in the interior and $O(h^p)$ near the boundary. In the accuracy analysis, the truncation error is partitioned into two parts: the interior truncation error and the boundary truncation error. It is straightforward to show by the energy method that the interior truncation error $O(h^{2p})$ results in an error $O(h^{2p})$ in the numerical solution. The boundary truncation error is often larger than the interior truncation error, and an important
3.3. Accuracy

Figure 3.5: Truncation error on the grid

feature of the boundary truncation error is depicted in Figure 3.5a, that is, it is only localized at a few grid points near the boundary and the number of grid points with the boundary truncation error $O(h^p)$ is independent of mesh refinements. The same is true for the truncation error near a grid interface as depicted in Figure 3.5b. This fact may weaken the effect of the boundary truncation error on the error in the numerical solution, and it can be expected that the error in the solution is $O(h^q)$ where $q > p$, which is often referred to as 'gain in convergence rate'.

The 'gain in convergence rate' phenomenon is well known and understood for first order hyperbolic equations [19], in which case one order is often recovered from the boundary truncation error. The accuracy analysis is based on Laplace transforming the semi–discretized equation in time and analyzing the determinant condition [21]. If the determinant condition is satisfied, we gain one order in the convergence rate for first order equations, and two orders for second order equations [61, 62]. For first order hyperbolic equations, the determinant condition is in many cases satisfied with a stable numerical scheme.

For the acoustic wave equation, we have found in [66] that the determinant condition is not satisfied even if the numerical scheme is stable by the energy method. In such cases, a detailed analysis of the solution to the Laplace transformed error equation is preformed to obtain how much is gained in the convergence rate.

The accuracy analysis for a problem in two space dimensions with non–periodic boundary conditions has not been done yet, and it is not easily generalized from the analysis for the one dimensional problem. In practice, the convergence rate for such problems is often conjectured based on the analysis for the corresponding one dimensional problem, and verified in numerical experiments. For the two dimensional acoustic wave equation solved
by the SBP–SAT method on a mesh with non–conforming grid interfaces, the convergence rate is one order lower than that in the case with only conforming grid interfaces. This is not surprising since the interpolation introduces an error $O(h^p)$ with a non–conforming grid interface. To guarantee stability, the corresponding penalty term is multiplied by $H^{-1}S^T \sim h^{-2}$. Therefore, the dominant truncation error is $O(h^{p-2})$. Since the number of grid points with the truncation error $O(h^{p-2})$ is finite and independent of $h$, its value in $L_2$ norm is one order higher than the pointwise truncation error, and we can hope to obtain more than the ’usual’ two orders gain. In the numerical experiments, a gain of three orders in convergence rate is observed. We refer to [67] for a detailed study.

Even though there are many advantages of using non–conforming grid interfaces in the mesh, we have to pay the cost of losing one order in convergence in the SBP–SAT framework, which may attenuate the efficiency of using a non–uniform mesh.
Chapter 4

Summary and future work

The work in this thesis leads to two manuscripts, where the SBP–SAT finite difference methods for the acoustic wave equation in the second order form are studied with an emphasis on the numerical treatments of boundary and grid interface conditions. In the first manuscript, the convergence rate of the proposed method is proved for the one dimensional problem with the Dirichlet or Neumann boundary conditions, and also the problem solved on a grid with a grid interface. The proof is also generalized to the two dimensional problems with a periodic boundary condition in one space dimension and non–periodic boundary condition in the other space dimension. The technique is based on Laplace transforming the error equation and analyzing the determinant condition. Two orders are recovered from the boundary and interface truncation error if the determinant condition is satisfied. However, in contrast to first order equations for which the determinant condition is in most cases satisfied for a stable numerical scheme, for second order equations it is less often satisfied even the scheme is stable by the energy method. In such cases, a detailed analysis of the determinant condition is performed to derive a sharp estimate of the error in the solution.

In the second manuscript, the SBP–SAT finite difference method applied to the two dimensional acoustic wave equation with non–conforming grid interface is discussed, and the numerical coupling is based on interpolation or projection techniques. In contrast to first order equations for which the norm–compatibility condition is sufficient to prove stability by the energy method, we show that for the acoustic wave equation an additional condition is needed. This condition is only satisfied for the second and fourth order accurate interpolation operators and projection operators. The numerical experiments, however, indicate that the scheme with the sixth order accurate interpolation operators is stable on a Cartesian grid but unphysical growth occurs on a curvilinear grid. The corresponding schemes with projection
operators are stable in all the experiments conducted in the manuscript. To fully understand the behaviour of the numerical methods, further stability and accuracy analysis is needed. The accuracy analysis in two space dimensions with non–periodic boundary conditions is not easily generalized from the analysis for one dimensional problems. When a non–conforming grid interface is present in the mesh, the dominant truncation error is localized at the corner in a low dimensional space. The analysis of its effect to the convergence property of the underlying numerical scheme has not been done, and will help greatly in the understanding of numerical interface treatments.

In the SBP–SAT framework for second order equations, the interpolation operators and projection operators allow a non–uniform mesh and make it possible to use local mesh refinement. An efficiency study in [67] demonstrates that in certain cases, it is beneficial to use non–conforming grid interfaces. However, the convergence rate is lowered by one order, compared with the case with only conforming grid interfaces. It is desirable to construct more accurate interpolation or projection operators, or develop a new numerical interface treatment to overcome the loss of accuracy so that it is practically useful for a general set of second order equations.

We have focused on numerical methods for the acoustic wave equation in this thesis. In the future, we will turn to the analysis of numerical schemes applied to the elastic wave equation, and investigate the convergence properties of such schemes on uniform and non–uniform meshes.
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Paper I
Convergence of summation–by–parts finite difference methods for the wave equation

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Abstract

In this paper, we consider finite difference approximations of the second order wave equation. We use finite difference operators satisfying the summation–by–parts property to discretize the equation in space. Boundary conditions and grid interface conditions are imposed by the simultaneous–approximation–term technique. Typically, the truncation error is larger at the grid points near a boundary or grid interface than that in the interior. Normal mode analysis can be used to analyze how the large truncation error affects the convergence rate of the underlying stable numerical scheme. If the semi–discretized equation satisfies a determinant condition, two orders are gained from the large truncation error. However, many interesting second order equations do not satisfy the determinant condition. We then carefully analyze the solution of the boundary system to derive a sharp estimate for the error in the solution and acquire the gain in convergence rate. The result shows that stability does not automatically yield a gain of two orders in convergence rate. The accuracy analysis is verified by numerical experiments.

Keywords: Second order wave equation, SBP-SAT, Finite difference, Accuracy, Convergence, Determinant condition, Normal mode analysis

AMS subject classifications: 65M06, 65M12, 65M15

1 Introduction

In many physical problems, such as acoustics, seismology, and electromagnetism, the underlying equations can be formulated as systems of second order time dependent hyperbolic partial differential equations. For wave propagation problems, it has been shown that high order accurate time marching methods as well as high order spatial discretization are more efficient to solve these problems on smooth domains [7, 9]. The major difficulties with high order spatial discretization are the numerical treatment of boundary conditions, grid interface conditions and interface conditions at material interfaces.

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High order finite difference methods have been widely used for wave propagation problems. We use summation-by-parts (SBP) finite difference operators \cite{11, 14, 18} to approximate spatial derivatives. In order to guarantee strict stability and maintain high accuracy, boundary conditions and grid interface conditions are imposed weakly by the simultaneous-approximation-term (SAT) technique \cite{2, 3, 12, 13}. This is often referred to as the SBP–SAT methodology, and a summary of it is made in \cite{4}. The energy method is used to determine the strength of the boundary enforcement and to derive an energy estimate for stability. Another candidate for the approximation of spatial derivatives is discontinuous Galerkin method, and it has been successfully used in \cite{5} for the wave equation.

In the SBP–SAT framework, accuracy analysis has drawn less attention than stability. A commonly used measure for accuracy is convergence rate, typically in $L_2$ norm. The convergence rate indicates how fast the error in the numerical solution approaches zero as the mesh size $h$ goes to zero. The error in the numerical solution is caused by truncation error. The truncation error near a boundary is often larger than that in the interior of the computational domain, but with the large boundary truncation error localized at a fixed number of grid points that is independent of mesh refinement. As a consequence, its effect to the convergence rate may be weakened. It is well-known that by applying directly the energy method to the error equation, $1/2$ order is gained in convergence. However, this convergence result is in many cases suboptimal. When using a finite difference method with mesh size $h$ to solve a first order hyperbolic partial differential equation, it is in many cases possible to show that $(p + 1)^{th}$ order convergence rate can be obtained if the boundary truncation error is $O(h^p)$ \cite{6, 7}. In other words, we gain one order in convergence rate. The technique used to analyze the effect of the boundary truncation error in \cite{6} is normal mode analysis. The idea is based on Laplace transforming the error equation in time. The error equation due to boundary truncation error can be formulated as a system of linear equations, which is referred to as the boundary system. A gain of one order in convergence rate follows if the boundary system is nonsingular for all $\text{Re}(s) > 0$, where $s$ is the dual variable of time in Laplace space. For such cases we use the same terminology as in \cite{8} and say that the boundary system satisfies the determinant condition. Also note that if a problem satisfies an energy estimate, the boundary system is nonsingular for $\text{Re}(s) > 0$. However, an energy estimate does in general not imply that the determinant condition is satisfied.

Also for many other systems the boundary truncation errors have less severe effect than predicted by energy estimates. In \cite{1} a parabolic problem is considered. Numerical experiments show a convergence rate $\min(2p, p + 2)$, where $p$ is the order of the boundary truncation error, while a careful deviation of the energy estimate yields $\min(2p, p + 3/2)$ as the convergence rate. This reaffirms that the energy estimate is an upper bound of the error, and indicates that the energy estimate is not always sharp.

A more general result on convergence rate is presented in \cite{17}, where it is shown that $k$ orders can be recovered from boundary truncation error for a partial differential equation with $k^{th}$ spatial derivatives. Parabolic, incomplete
parabolic and second order hyperbolic partial differential equations are considered, and for these equations we call $\min(2p, p + 2)$ the optimal convergence rate. The condition for the optimal convergence is formulated in terms of a new stability concept, pointwise stability, but the underlying analysis of the optimal convergence is based on the determinant condition, and therefore the approach cannot be applied when the boundary system is singular at the origin.

When using SBP–SAT finite difference method to solve second order hyperbolic partial differential equations, there are many cases that the boundary system does not satisfy the determinant condition. In this paper, we aim at filling the gap in the study of convergence rate for such problems. We use the wave equation in second order form as our model problem. In particular, we consider problems with Dirichlet boundary condition, Neumann boundary condition and grid interface condition. We refer to them as the Dirichlet problem, the Neumann problem and the interface problem, respectively. By analyzing the error equation, we obtain a boundary system of linear equations. If the determinant condition is satisfied, we would get the optimal convergence rate as shown in [8, Ch.12]. If the determinant condition is not satisfied on the imaginary axis, [8, 17] are not applicable and one has to carefully derive an estimate for the solution of the boundary system to see how much is gained in convergence rate.

In this paper, we find that 1) an energy estimate for the second order wave equation does not imply an optimal convergence rate; 2) the determinant condition is not necessary for an optimal convergence rate; 3) if there is an energy estimate but the determinant condition is not satisfied, there can be an optimal gain of order 2, or a non–optimal gain of order 1, or only a 1/2 order gain that is given by the energy estimate. We demonstrate how to analyze the boundary system to determine the accuracy gain.

More specifically, for the Dirichlet problem, the boundary system is singular or nonsingular depending on the value of the penalty parameter in SAT. In this case, the optimal convergence rate is only obtained when the determinant condition is satisfied. For the Neumann and the interface problems, the determinant condition is not satisfied even though the schemes are stable. We will analyze the boundary system, and show how much is gained in convergence in those cases. The analysis agrees well with numerical experiments. In [15, 16], the same technique is also used to prove optimal convergence rate for Schrödinger equation.

The structure of this paper is as follows. We start in §2 with the SBP–SAT method applied to the one dimensional wave equation with Dirichlet boundary condition. We apply the energy method and normal mode analysis, and derive results that correspond to the second, fourth and sixth order schemes. We then discuss the Neumann problem in §3. In §4, we consider one dimensional wave equation on a grid with a grid interface. We extend the analysis to two dimensions in §5. In §6, we perform numerical experiments. The computational convergence results support the accuracy analysis. The conclusions are drawn in §7.
2 One dimensional wave equation with Dirichlet boundary condition

To describe the properties of the equation and the numerical methods, we need the following definitions. Let \( w_1(x) \) and \( w_2(x) \) be real–valued functions in \( L^2[a_1,a_2] \). The inner product is defined as \( (w_1,w_2) = \int_{a_1}^{a_2} w_1 w_2 dx \). The corresponding norm is \( \|w_1\|^2 = (w_1,w_1) \).

The second order wave equation in one dimension takes the form
\[
U_{tt} = U_{xx} + F, \quad x \in [0,1], \quad t \geq 0,
\]
\[
U(x,0) = f^1(x), \quad U_t(x,0) = f^2(x).
\]
(1)

where \( F \) is a forcing term. We consider the half line problem with Dirichlet boundary condition:
\[
U(0,t) = g(t).
\]
(2)

The forcing function \( F \), the initial data \( f^1, f^2 \) and the boundary data \( g \) are compatible smooth functions with compact support. For the problem (1) in a bounded domain, there is one boundary condition at each boundary. For the half line problem in consideration, the right boundary condition is substituted by requiring that the \( L^2 \) norm of the solution is bounded, i.e. \( \|U(\cdot,t)\| < \infty \).

The problem (1)–(2) is well–posed if there is an energy estimate with \( g(t) = 0 \) and the problem is boundary stable. In [10, Definition 2.3], it is defined that the problem (1)–(2) is boundary stable if with \( f^1 = f^2 = 0 \) and \( F = 0 \) there are constants \( \eta_0 \geq 0, K > 0 \) and \( \alpha > 0 \) independent of \( g \) such that for all \( \tilde{\eta} > \eta_0 \), \( T \geq 0 \),
\[
\int_0^T e^{-2\tilde{\eta}t} |u(0,t)|^2 dt \leq \frac{K}{\tilde{\eta}^\alpha} \int_0^T e^{-2\eta_0t} |g(t)|^2 dt.
\]

It is obvious that (1) is boundary stable with Dirichlet boundary condition. To derive an energy estimate, we multiply Equation (1) by \( U_t \) and integrate by parts. With homogeneous Dirichlet boundary condition \( g(t) = 0 \), we obtain
\[
\frac{d}{dt} \sqrt{E} \leq \|F\|,
\]
where \( E = \|U_t\|^2 + \|U_x\|^2 \) is the continuous energy. The energy estimate follows from Gronwall’s lemma
\[
\sqrt{E} \leq \sqrt{\|f^1_x\|^2 + \|f^2_x\|^2} + \int_0^t \|F(\cdot,z)\| dz.
\]
(3)

Therefore, problem (1)–(2) is well–posed.

Next, we introduce the equidistant grid \( x_i = ih, \ i = 0,1,2, \ldots \), and a grid function \( u_i(t) \approx U(x_i,t) \). Furthermore, let \( u(t) = [u_0(t),u_1(t), \ldots]^T \). We also define an inner product and norm for the grid functions \( a \) and \( b \) in \( \mathcal{R} \) as \((a,b)_H = a^T H b\) and \( \|a\|_H^2 = a^T H a \), respectively, where \( a^T \) denotes the transpose of \( a \) and \( H \) is a positive definite operator in the space of grid functions. An SBP operator approximates a derivative, and mimics the property of the continuous integration-by-parts via the inner product and norm defined above.
Table 1: $\alpha_{2p}$ values

<table>
<thead>
<tr>
<th>$2p$</th>
<th>2</th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_{2p}$</td>
<td>0.4</td>
<td>0.2508560249</td>
<td>0.1878715026</td>
<td>0.0015782259</td>
<td>0.0351202265</td>
</tr>
</tbody>
</table>

In this paper, we use the diagonal norm SBP operator $D$ approximating second order derivative, i.e. $D \approx \frac{\partial^2}{\partial x^2}$. The order of accuracy is denoted by $2p$, $p = 1, 2, 3, 4, 5$. For a $2p^{th}$ order diagonal norm SBP operator [11, 14], the error for the approximation of the spatial derivative is $O(h^{2p})$ in the interior, and $O(h^{p})$ near the boundary. The SBP operator can be written as $D = H^{-1}(-A + BS)$, where $H$ is diagonal and positive definite, $A$ is symmetric positive semi-definite and $B = diag(-1, 0, 0, \cdots)$. $S$ is a one sided approximation of the first derivative at the boundary with the order of accuracy $p + 1$. The elements in $D$ are proportional to $1/h^2$ while the elements in $H^{-1}$ and $S$ are proportional to $1/h$. Another version of the SBP operators are constructed with block norms, see [11, 14].

We use the SAT technique to impose the Dirichlet boundary condition weakly. The semi-discretized equation corresponding to (1) and (2) with homogeneous boundary data reads:

$$u_{tt} = Du - H^{-1}S^TE_0u - \frac{\tau}{h}H^{-1}E_0u + F_g,$$

where $e_0 = [1, 0, 0, \cdots]^T$, $E_0 = e_0e_0^T$ and $F_g$ is the grid function corresponding to $F(x, t)$. On the right hand side, the first term is an approximation of $U_{xx}$, while the second and third terms impose weakly the boundary condition $U(0, t) = 0$. They act as penalty terms draggning the numerical solution at the boundary towards zero so that the boundary condition is simultaneously approximated. In general, the boundary condition is not satisfied exactly. The penalty parameter $\tau$ is to be determined so that an energy estimate of the discrete solution exists, which ensures stability.

### 2.1 Stability

In [2, 12, 13], it is shown that the operator $A$ can be written as

$$A = h\alpha_{2p}(E_0S)^T E_0S + \tilde{A},$$

where $\alpha_{2p} > 0$ is as large as possible and $\tilde{A}$ is symmetric positive semi-definite. This is often called the borrowing trick. We use the technique in [12] to compute the values of $\alpha_{2p}$ and list the results in Table 1.

Multiplying Equation (4) by $u_t^T H$ from the left, with (5) we obtain

$$\frac{d}{dt}\left(\|u_t\|_H^2 + \|u\|_A^2 + \left(\sqrt{h\alpha_{2p}(BSu)_0} - \frac{1}{\sqrt{h\alpha_{2p}}} u_0\right)^2 + \left(\tau - \frac{1}{\alpha_{2p}}\right) \frac{u_0^2}{h}\right)_{E_h} = 2u_t HF_g.$$
For $\tau \geq \frac{1}{\alpha_{2p}}$, we have $E_h \geq 0$. In this case, $\|u\|^2_h := E_h$ is a discrete energy, and $\|\cdot\|_h$ is the corresponding discrete energy norm. We then obtain the discrete energy estimate

$$\sqrt{E_h} \leq \sqrt{E_{h,0}} + \int_0^t \|F_g(\cdot, z)\|_{Hdz},$$

where $E_{h,0}$ is the initial discrete energy. Clearly, stability is ensured if $\tau \geq \frac{1}{\alpha_{2p}}$.

Remark It is possible to include the term $\|u\|^2_H$ in the discrete energy $E_h$. A similar energy estimate holds [8]. This is useful when comparing the numerical results with the theoretical analysis.

2.2 Accuracy analysis by the energy estimate

Assuming that the continuous problem has a smooth solution $U(x,t)$, we can derive the error equation for the pointwise error $\xi_j = U(x_j, t) - u_j(t)$. The error equation corresponding to (4) is

$$\xi_{tt} = D\xi - H^{-1}S^T E_0\xi - \frac{\tau}{h} H^{-1} E_0\xi + T^{2p},$$

(6)

where $\|\xi(t)\|_h < \infty$, $T^{2p}$ is the truncation error and $2p$ is the accuracy order of the SBP operator. The first $m$ components of $T^{2p}$ are of order $O(h^p)$, and all the other components are of order $O(h^{2p})$. For $2p = 2, 4, 6, 8, 10$, the corresponding $m$ values are $1, 1, 3, 5, 7$. In the analysis, we only consider the leading term of the truncation error. We introduce the interior truncation error $T^{2p,I}$, and the boundary truncation error $T^{2p,B}$ such that

$$T^{2p} = h^p T^{2p,I} + h^{2p} T^{2p,B},$$

where $T^{2p,I}$ and $T^{2p,B}$ are independent of $h$, but depend on the derivatives of $U$. We have

$$T^{2p,I}_i \begin{cases} = 0 & 0 \leq i \leq m-1 \\ \neq 0 & i > m-1 \end{cases} \quad \text{and} \quad T^{2p,B}_i \begin{cases} = 0 & i \geq m-1 \\ \neq 0 & 0 \leq i \leq m-1 \end{cases}.$$

Since the number of grid points with the large truncation error $O(h^p)$ is finite and independent of $h$, we have

$$\|T^{2p}\|_h^2 = h(h^{4p} \sum_{i=m}^{\infty} |T^{2p,I}_i|^2 + h^{2p} \sum_{i=0}^{m-1} |T^{2p,B}_i|^2) \leq K_I h^{4p} + K_B h^{2p+1}.$$ 

For $2p = 2, 4, 6, 8, 10$ and small $h$, the first term is much smaller than the second one. Thus, we have $\|T^{2p}\|_h \leq \tilde{K}_B h^{p+1/2}$. By applying energy method to the error equation (6), we obtain

$$\|\xi\|_h \leq C_e h^{p+1/2}.$$ 

This means that by the energy method we can only prove a gain in accuracy order of 1/2. Therefore, the convergence rate is at least $p + \frac{1}{2}$ if the numerical scheme is stable, that is if $\tau \geq \tau_{2p}$. 
2.3 Normal mode analysis for the boundary truncation error

To derive a sharp estimate, we partition the pointwise error into two parts, the interior error $\epsilon^I$ and the boundary error $\epsilon$, such that $\xi = \epsilon^I + \epsilon$. $\epsilon^I$ is the error due to the interior truncation error, and $\epsilon$ is the error due to the boundary truncation error. $\epsilon^I$ can be estimated by the energy method, yielding

$$\|\| \epsilon^I \|_h \leq C_I h^{2p}. \tag{7}$$

where $C_I$ is a constant independent of $h$.

We perform a normal mode analysis to analyze the boundary truncation error $\epsilon$ for second, fourth and sixth order SBP-SAT scheme. The boundary error equation is

$$\epsilon_{tt} = D\epsilon - H^{-1} S^T E_0 \epsilon - \frac{\tau}{h} H^{-1} E_0 \epsilon + h^p \tilde{T}_{2p}. \tag{8}$$

where $\|\epsilon\|_h < \infty$. In the analysis of $\epsilon$, we take the Laplace transform in time of (8),

$$s^2 \hat{\epsilon} = D\hat{\epsilon} - H^{-1} S^T E_0 \epsilon - \frac{\tau}{h} H^{-1} E_0 \epsilon + h^p \tilde{T}_{2p}. \tag{9}$$

for $\text{Re}(s) > 0$, where $\hat{\cdot}$ denotes the variable in the Laplace space. Let $\tilde{s} = sh$. After multiplying $h^2$ on both sides of (9), we obtain

$$\tilde{s}^2 \hat{\epsilon} = h^2 D\hat{\epsilon} - h^2 H^{-1} S^T E_0 \epsilon - \tau h H^{-1} E_0 \epsilon + h^{p+2} \tilde{T}_{2p}. \tag{10}$$

Note that the first three terms in the right hand side of (10) are $h$-independent.

By assumption the true solution $U(x, t)$ is smooth. As a consequence, $|\tilde{T}_{2p}(s)|$ decreases fast for large $|s|$. Convergence rate is an asymptotic behaviour as the mesh size $h$ approaches zero. Therefore, we need to investigate the solution of (10) as $\tilde{s}$ approaches zero. In the analysis, we assume $|s| \leq K$ and consider $\text{Re}(s) \geq \eta > 0$, where $K$ and $\eta$ are some positive constants. Equivalently, $|\tilde{s}| \ll 1$ and $\text{Re}(\tilde{s}) \geq \eta h$. If the semi-discretized equation is stable, the Laplace transformed problem is nonsingular for $\text{Re}(\tilde{s}) > 0 \ [8]$.

There are essentially two steps in the normal mode analysis. Firstly, by a detailed analysis of the error equation (10), we obtain an estimate for $\|\epsilon\|_h$ in the Laplace space. Then we use Parseval’s relation to derive an estimate for the error in the physical space of the form

$$\sqrt{\int_0^{t_f} \|\epsilon(\cdot, t)\|_h^2 dt} \leq Ch^q, \tag{11}$$

where $C$ depends only on $\eta$, the final time $t_f$ and the derivatives of the true solution $U$. The results for the Dirichlet problem are summarized in Theorem 2.1.

**Theorem 2.1.** For the second, fourth and sixth order stable SBP-SAT approximations of the second order wave equation (1-2) on a half line with Dirichlet boundary condition, the rates $q$ in (11) depend on $\tau$, and are listed in Table 2.
In §6, we present results from numerical experiments, which agree well with the theoretical results in Table 2. After some preliminaries we will prove Theorem 2.1 for $2p = 2, 4$ and $6$ in §2.3.1, 2.3.2 and 2.3.3, respectively. In the proof, we will show that the determinant condition is satisfied if $\tau > \tau_{2p}$ but not satisfied if $\tau = \tau_{2p}$. In addition, the determinant condition is necessary for the optimal convergence rate.

To begin with, we note that sufficiently far away from the boundary, the two penalty terms and the boundary truncation error in (10) are not present. The coefficients in $D$ correspond to that in the standard central finite difference scheme. We have

\begin{align}
2p = 2: & \quad s^2 \hat{\epsilon}_j = D_+D_-\hat{\epsilon}_j, \quad j = 3, 4, 5, \ldots, \\
2p = 4: & \quad s^2 \hat{\epsilon}_j = (D_+D_- - \frac{1}{12}(D_+D_-)^2)\hat{\epsilon}_j, \quad j = 4, 5, 6, \ldots, \\
2p = 6: & \quad s^2 \hat{\epsilon}_j = (D_+D_- - \frac{h^2}{12}(D_+D_-)^2 + \frac{h^4}{90}(D_+D_-)^3)\hat{\epsilon}_j, \quad j = 5, 6, 7, \ldots,
\end{align}

where

\[
D_+\hat{\epsilon}_j = \frac{\hat{\epsilon}_{j+1} - \hat{\epsilon}_j}{h} \quad \text{and} \quad D_-\hat{\epsilon}_j = \frac{\hat{\epsilon}_j - \hat{\epsilon}_{j-1}}{h}.
\]

The corresponding characteristic equations are

\begin{align}
2p = 2: & \quad \kappa^2 - (2 + \hat{s}^2)\kappa + 1 = 0, \\
2p = 4: & \quad \kappa^4 - 16\kappa^3 + (30 + 12\hat{s}^2)\kappa^2 - 16\kappa + 1 = 0, \\
2p = 6: & \quad 2\kappa^6 - 27\kappa^5 + 270\kappa^4 - (180\hat{s}^2 + 490)\kappa^3 + 720\kappa^2 - 27\kappa + 2 = 0.
\end{align}

It is easy to verify by von Neumann analysis that the interior numerical scheme is stable when applied to the corresponding periodic problem. From Lemma 12.1.3 in [8, pp. 379], it is straightforward to prove that there is no root with $|\kappa| = 1$ for $\text{Re}(s) > 0$. We will need the following specifics for the roots.

**Lemma 2.2.** For $2p = 2, 4, 6$, the number of admissible roots of (13) satisfying $|\kappa| < 1$ for $\text{Re}(\hat{s}) > 0$ is 1, 2, 3, respectively. In the vicinity of $\hat{s} = 0$, they are
Proof. \(2p = 2\): Equation (13a) has two roots: \(\kappa_{1,2} = 1 + \frac{1}{2} \hat{s}^2 \pm \frac{1}{2} \sqrt{\hat{s}^4 + 4 \hat{s}^2} \). We find by Taylor expansion at \(\hat{s} = 0\) that \(\kappa_1 = 1 - \hat{s} + \mathcal{O}(\hat{s}^2)\) and \(\kappa_2 = 1 + \hat{s} + \mathcal{O}(\hat{s}^2)\). Thus, the admissible root is \(\kappa_1 = 1 - \hat{s} + \mathcal{O}(\hat{s}^2)\).

\(2p = 4\): Equation (13b) has four roots:
\[
\begin{align*}
\kappa_1 &= \sqrt{24 - 3\hat{s} - 8\sqrt{9 - 3\hat{s}^2} - \sqrt{9 - 3\hat{s}^2} + 4}, \\
\kappa_2 &= 4 - \sqrt{9 - 3\hat{s}^2} - \sqrt{24 - 3\hat{s} - 8\sqrt{9 - 3\hat{s}^2}}, \\
\kappa_3 &= \sqrt{9 - 3\hat{s}^2} - \sqrt{8\sqrt{9 - 3\hat{s}^2} - 3\hat{s} + 24 + 4}, \\
\kappa_4 &= \sqrt{8\sqrt{9 - 3\hat{s}^2} - 3\hat{s} + 24 + \sqrt{9 - 3\hat{s}^2} + 4}.
\end{align*}
\]

We find by Taylor expansion at \(\hat{s} = 0\) that
\[
\begin{align*}
\kappa_1 &= 1 - \hat{s} + \mathcal{O}(\hat{s}^2), \\
\kappa_2 &= 7 - 4\sqrt{3} + \mathcal{O}(\hat{s}^2), \\
\kappa_3 &= 7 + 4\sqrt{3} + \mathcal{O}(\hat{s}^2), \\
\kappa_4 &= 1 + \hat{s} + \mathcal{O}(\hat{s}^2).
\end{align*}
\]

Thus, the admissible roots are \(\kappa_1 = 1 - \hat{s} + \mathcal{O}(\hat{s}^2)\) and \(\kappa_2 = 7 - 4\sqrt{3} + \mathcal{O}(\hat{s}^2)\).

\(2p = 6\): (13c) is a six order equation. There is no formula for general six order equations over the rationals in terms of radicals. We solve numerically equation (13c) with \(\hat{s} = 0\), and then analyze the six roots by perturbation theory to find out their dependence on \(\hat{s}\). The three admissible roots are given by (14c).

\[\square\]

**Lemma 2.3.** Consider \(|\hat{s}| < 1\) and \(\text{Re}(\hat{s}) \geq \eta h > 0\). For \(2p = 2, 4, 6\) the admissible roots \(\kappa_1(\hat{s})\) satisfy
\[1 - |\kappa_1(\hat{s})|^2 \geq 2\text{Re}(\hat{s}) + \mathcal{O}(|\hat{s}|^2).\]

**Proof.** Let \(\hat{s} = x + iy\) where \(x, y\) are real numbers. Then \(|x| \geq \eta h\).
\[
1 - |\kappa_1(\hat{s})|^2 = 1 - |1 - \hat{s} + \mathcal{O}(\hat{s}^2)|^2 \\
\geq 1 - |1 - \hat{s}|^2 + \mathcal{O}(|\hat{s}|^2) \\
= 1 - |1 - x - y^2|^2 + \mathcal{O}(|\hat{s}|^2) \\
= 2x - x^2 - y^2 + \mathcal{O}(|\hat{s}|^2) \\
= 2\text{Re}(\hat{s}) + \mathcal{O}(|\hat{s}|^2).
\]

\[\square\]

By Lemma 2.3, we obtain \(\frac{1}{1 - |\kappa(\hat{s})|^2} \leq \frac{1}{2\eta h}\) to the leading order. We will use this inequality to estimate \(\|\hat{\epsilon}\|_h\).
2.3.1 Proof of Theorem 2.1 for the second order scheme

Away from the boundary, equation (10) is simplified to (12a), which is a recursion relation for \( \hat{e}_j \). A general solution of (12a) can be written as

\[
\hat{e}_j = \sigma \kappa_1^{j-2}, \quad j = 2, 3, 4, \ldots,
\]

where \( \kappa_1 \) is obtained from (14a) and \( \sigma \) is an unknown in the boundary system. In the following, we derive the boundary system and investigate its solution near \( \tilde{s} = 0 \) to obtain an estimate of the error in the Laplace space. The first three rows of (10) are affected by the penalty terms. They are

\[
\begin{align*}
\tilde{s}^2 \hat{e}_0 &= \hat{e}_0 - 2 \hat{e}_1 + \hat{e}_2 + 3 \hat{e}_0 - 2\tau \hat{e}_0 + h^3 \tau^2 B, \\
\tilde{s}^2 \hat{e}_1 &= \hat{e}_0 - 2 \hat{e}_1 + \hat{e}_2 - 2 \hat{e}_0, \\
\tilde{s}^2 \hat{e}_2 &= \hat{e}_1 - 2 \hat{e}_2 + \hat{e}_3 - \frac{1}{2} \hat{e}_0.
\end{align*}
\]

By Taylor expansion, it is straightforward to derive \( \hat{T}_0^2 B = -\hat{U}_{xxx}(0, s) \) to the leading order. We write (16) in the matrix vector multiplication form with the help of (15), and obtain the boundary system

\[
\begin{bmatrix}
-1 & \tilde{s}^2 - 4 + 2\tau & 2 \\
-1 & 1 & \tilde{s}^2 + 2 \\
\kappa_1 - 2 - \tilde{s}^2 & \frac{1}{2} & 1
\end{bmatrix}
\begin{bmatrix}
\sigma \\
\hat{e}_0 \\
\hat{e}_1
\end{bmatrix}
= h^3
\begin{bmatrix}
-\hat{U}_{xxx}(0, s) \\
0 \\
0
\end{bmatrix}.
\]

Next, we investigate the invertibility of \( C_{2D}(\tilde{s}, \tau) \) in a vicinity of \( \tilde{s} = 0 \) to derive an estimate for \( |\Sigma_{2D}| \), where \( |\cdot| \) denote the standard Euclidean norm of vectors and matrices. We note that

\[
C_{2D}(0, \tau) =
\begin{bmatrix}
-1 & -4 + 2\tau & 2 \\
-1 & 1 & 2 \\
-1 & \frac{1}{2} & 1
\end{bmatrix}.
\]

The determinant of \( C_{2D}(0, \tau) \) is given by \( \det(C_{2D}(0, \tau)) = 5 - 2\tau \). Clearly, \( C_{2D}(0, \tau) \) is singular if \( \tau = 2.5 \) and nonsingular otherwise. The stability condition is \( \tau \geq \tau_2 = 2.5 \).

In the case \( \tau > \tau_2 \), \( C_{2D}(0, \tau) \) is nonsingular. By the continuity of \( C_{2D}(\tilde{s}, \tau) \), for any \( \gamma > 1 \) and sufficiently small \( h \) we have \( |C_{2D}^{-1}(\tilde{s}, \tau)| \leq \gamma |C_{2D}^{-1}(0, \tau)| \). Thus, \( |\Sigma_{2D}| \leq \gamma |C_{2D}^{-1}(0, \tau)||\hat{T}_v^2 B|h^3 \). Therefore, we have \( |\sigma|^2 \leq K_\sigma |\hat{U}_{xxx}(0, s)|^2 h^6 \) and \( \sum_{i=0}^\infty |\hat{e}_i|^2 \leq K_i |\hat{U}_{xxx}(0, s)|^2 h^6 \), where \( K_\sigma \) and \( K_i \) are constants independent of \( h \). In L2 norm, we have

\[
\left\| \hat{e} \right\|_h^2 = h \sum_{i=0}^\infty |\hat{e}_i|^2 + h |\sigma|^2 \sum_{i=0}^\infty |\kappa_1|^{2i} = h \left\| \hat{e} \right\|_{2,h}^2 + h |\sigma|^2 \frac{1}{1 - |\kappa_1|^2}.
\]

\[
\left\| \hat{e} \right\|_{1,h}^2 = \left\| \hat{e} \right\|_{2,h}^2 + h |\sigma|^2 \frac{1}{1 - |\kappa_1|^2}.
\]
By Lemma 2.3, we have \( \| \hat{\epsilon} \|_h^2 = h|\sigma|^2 \frac{1}{1-|\kappa_1|^2} \leq \frac{K_\sigma}{2\eta} |\hat{U}_{xxx}(0, s)|^2 h^6 \). The first term can be bounded as \( \| \hat{\epsilon} \|_{B,h}^2 = h \sum_{i=0}^1 |\hat{\epsilon}_i|^2 \leq K_\epsilon |\hat{U}_{xxx}(0, s)|^2 h^7 \ll \| \hat{\epsilon} \|_{I,h}^2 \) for small \( h \). Thus, to the leading order,

\[
\| \hat{\epsilon} \|_h^2 \leq \frac{K_\sigma}{2\eta} |\hat{U}_{xxx}(0, s)|^2 h^6,
\]

where \( K_\sigma \) is a constant independent of \( h \). By Parseval’s relation, we have

\[
\int_0^\infty e^{-2nt} \| \hat{\epsilon} \|_h^2 dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} \| \hat{\epsilon}(\eta + i\xi) \|_h^2 d\xi \\
\leq \frac{K_\sigma h^6}{4\pi\eta} \int_{-\infty}^{\infty} |\hat{U}_{xxx}(0, \eta + i\xi)|^2 d\xi \\
= \frac{K_\sigma h^6}{2\eta} \int_0^\infty e^{-2nt} |U_{xxx}(0, t)|^2 dt.
\]

Note that in the above, we use Parseval’s relation twice. By arguing that the future cannot affect the past, we can replace the upper limit of the integrals on both sides by a finite time \( t_f \). Since

\[
\int_0^{t_f} e^{-2nt} \| \hat{\epsilon} \|_h^2 dt \leq \int_0^{t_f} e^{-2nt} \| \hat{\epsilon} \|_h^2 dt, \\
\int_0^{t_f} e^{-2nt} |U_{xxx}(0, t)|^2 dt \leq \int_0^{t_f} |U_{xxx}(0, t)|^2 dt,
\]

we obtain

\[
\sqrt{\int_0^{t_f} \| \hat{\epsilon} \|_h^2 dt} \leq h^3 \sqrt{\frac{K_\sigma e^{2nt_f}}{2\eta} \int_0^{t_f} |U_{xxx}(0, t)|^2 dt}.
\]

Thus, the boundary error is \( O(h^3) \). In this case, the interior error is \( O(h^2) \) by (7), which is the dominating source of error. Therefore, the overall convergence rate is 2.

In the case \( \tau = \tau_2, C_{2D}(0, \tau) \) is singular, and the above analysis is not valid. By the energy estimate the convergence rate is \( p + \frac{1}{2} = 1.5 \).

### 2.3.2 Proof of Theorem 2.1 for the fourth order scheme

Away from the boundary, the solution of (10) is

\[
\hat{\epsilon}_j = \sigma_1 \kappa_1^{j-2} + \sigma_2 \kappa_2^{j-2}, \quad j = 2, 3, 4, \ldots,
\]

where \( \kappa_1, \kappa_2 \) are obtained from (14b), and \( \sigma_1, \sigma_2 \) will be determined by the boundary system. The first four rows of (10) are affected by the penalty terms.
They are
\[
\begin{align*}
s^2 \hat{\epsilon}_0 &= \left( \frac{122 - 48\tau}{17} \right) \hat{\epsilon}_0 - 5\hat{\epsilon}_1 + 4\hat{\epsilon}_2 - \hat{\epsilon}_3 + h^4 \hat{T}_0^{4,B}, \\
s^2 \hat{\epsilon}_1 &= -\frac{85}{59} \hat{\epsilon}_0 - 2\hat{\epsilon}_1 + \hat{\epsilon}_2 + h^4 \hat{T}_1^{4,B}, \\
s^2 \hat{\epsilon}_2 &= \frac{68}{43} \hat{\epsilon}_0 + \frac{59}{43} \hat{\epsilon}_1 - \frac{110}{43} \hat{\epsilon}_2 + \frac{59}{43} \hat{\epsilon}_3 - \frac{4}{43} \hat{\epsilon}_4 + h^4 \hat{T}_2^{4,B}, \\
s^2 \hat{\epsilon}_3 &= -\frac{17}{49} \hat{\epsilon}_0 + \frac{59}{49} \hat{\epsilon}_1 - \frac{118}{49} \hat{\epsilon}_2 + \frac{64}{49} \hat{\epsilon}_3 - \frac{4}{49} \hat{\epsilon}_4 + h^4 \hat{T}_3^{4,B}.
\end{align*}
\]
By Taylor expansion, we have
\[
\begin{align*}
\hat{T}_0^{4,B} &= \frac{11}{12} \hat{U}_{xxxx}(0, s), \\
\hat{T}_1^{4,B} &= -\frac{1}{12} \hat{U}_{xxxx}(0, s), \\
\hat{T}_2^{4,B} &= \frac{5}{516} \hat{U}_{xxxx}(0, s), \\
\hat{T}_3^{4,B} &= \frac{11}{588} \hat{U}_{xxxx}(0, s)
\end{align*}
\]
to the leading order. With \( \hat{s} = 0 \), the boundary system follows from (17)–(18)
\[
C_{4D}(0, \tau) \Sigma_{4D} = h^4 \hat{T}_v^{4,B},
\]
where \( \Sigma_{4D} = [\sigma_1, \sigma_2, \hat{\epsilon}_0, \hat{\epsilon}_1]^T \), \( \hat{T}_v^{4,B} = [\hat{T}_0^{4,B}, \hat{T}_1^{4,B}, \hat{T}_2^{4,B}, \hat{T}_3^{4,B}]^T \) and \( C_{4D}(0, \tau) \) is given in Appendix 1. We solve for \( \det(C_{4D}(0, \tau)) = 0 \), and obtain \( \tau = \frac{2(4834\sqrt{3}+9569)}{177(8\sqrt{3}+37)} \approx 3.986350342 \). Recall that the stability condition is \( \tau \geq \tau_4 \approx 3.986350342 \).

In the case \( \tau > \tau_4 \), \( C_{4D}(0, \tau) \) is nonsingular. Similarly to the second order case in \( \S 2.3.1 \), we obtain to leading order
\[
\| \hat{\epsilon} \|^2_h \leq \frac{K_{\sigma_1}}{2\eta} |\hat{U}_{xxxx}(0, s)|^2 h^8.
\]
By Parseval’s relation and by arguing that the future cannot affect the past, we obtain
\[
\sqrt{\int_0^{t_f} \| \hat{\epsilon} \|^2_h dt} \leq h^4 \sqrt{\frac{K_{\sigma_1} e^{2\eta t_f}}{2\eta} \int_0^{t_f} |U_{xxxx}(0, t)|^2 dt}.
\]
Thus, the boundary error is \( \mathcal{O}(h^4) \). In this case, the interior error is also \( \mathcal{O}(h^4) \) given by (7). Therefore, the convergence rate is 4.

In the case \( \tau = \tau_4 \), \( C_{4D}(0, \tau) \) is singular. By the energy estimate, the convergence rate is \( p + \frac{1}{2} = 2.5 \).

### 2.3.3 Proof of Theorem 2.1 for the sixth order scheme

Away from the boundary, the solution of (10) is
\[
\hat{\epsilon}_j = \sigma_1 \kappa_1^{j-3} + \sigma_2 \kappa_2^{j-3} + \sigma_3 \kappa_3^{j-3}, \quad j = 3, 4, 5, \ldots
\]
where \( \kappa_1, \kappa_2, \kappa_3 \) are obtained from (14c), and \( \sigma_1, \sigma_2, \sigma_3 \) are determined by the boundary system. Near the boundary, the first six rows of (10) are affected by
the penalty terms. In the same way as for the second and fourth order method, we obtain the boundary system in $\Sigma_{6D} = [\hat{e}_0, \hat{e}_1, \hat{e}_2, \sigma_1, \sigma_2, \sigma_3]^T$

$$C_{6D}(\tilde{s}, \tau)\Sigma_{6D} = h^5\tilde{T}^{6,B}_v,$$

where $C_{6D}(\tilde{s}, \tau)$ is given in Appendix 1. We find that $C_{6D}(0, \tau)$ is singular if $\tau = \tau_6$, and nonsingular otherwise. When $\tau > \tau_6$, we use Taylor expansion to express $T_v^{6,B}$ in terms of the derivatives of the true solution $U$, and Lemma 2.3 to derive an estimate for (19). The boundary error is $O(h^5)$. In this case, the interior error is $O(h^6)$ given by (7). Thus, the convergence rate is 5.

When $\tau = \tau_6$, the convergence rate $p + \frac{1}{2} = 3.5$ is given by the energy estimate.

3 One dimensional wave equation with Neumann boundary condition

Next, we consider an example which never satisfies the determinant condition, but nonetheless exhibits optimal convergence. We consider Equation (1) with Neumann boundary condition

$$U_x(0, t) = g(t).$$

(20)

We use the same assumption of the data as for the Dirichlet problem. With homogeneous Neumann boundary condition $g(t) = 0$ we get an energy estimate identical to the one for the Dirichlet problem (3). To prove well-posedness, we also need to show that the equation is boundary stable. Boundary stability for the Neumann problem is proved in [10, Theorem 3.8] by Laplace transform technique.

3.1 Stability

To discretize the equation in space, we use the grid and grid functions introduced for the Dirichlet problem. The semi–discretized equation of the Neumann problem is

$$u_{tt} = Du + H^{-1}E_0Su + F_g.$$  

(21)

On the right hand side of (21), the first term approximates $U_{xx}$ and the second term imposes weakly the boundary condition $U_x(0, t) = 0$. Since we consider a half line problem, the SBP operator $D$ can be written as $D = H^{-1}(-M - E_0S)$. As a consequence, the semi–discretization (21) can be written as

$$u_{tt} = -H^{-1}Mu + F_g.$$  

(22)

Multiplying Equation (22) by $u_t^T H$ from the left, we obtain

$$\frac{d}{dt} \left( \|u_t\|_H^2 + \|u\|_M^2 \right) = 2u_t HF.$$
The discrete energy $E_{Neu}^k = ||u||_{Neu}^k := ||u_t||_H^2 + ||u||_H^2$ is bounded as
\[
\sqrt{E_{Neu}^k} \leq \sqrt{E_{Neu,h0}^k} + \int_0^t \|F_g(\cdot, z)\|_H dz. \tag{23}
\]
(23) is the energy estimate.

3.2 Accuracy

Define the pointwise error as $\xi_j = U(x_j, t) - u_j(t)$. The error equation corresponding to (22) is
\[
\xi_{tt} = -H^{-1} M \xi + T^{2p,Neu}, \tag{24}
\]
where $||\xi||_h < \infty$, $T^{2p,Neu}$ is the truncation error and $2p$ is the accuracy order of the SBP operator. In the same way as for the Dirichlet problem, by applying the energy method to the error equation (24), we obtain an estimate
\[
|||\xi|||_{Neu}^k \leq C_{Neu} h^{p+1/2},
\]
where $C_{Neu}$ is a constant independent of $h$. This means that the convergence rate of (22) is at least $p + 1/2$. In the following, we use normal mode analysis to derive a sharp bound of the error, which agrees well with the results from numerical experiments.

Similar to the Dirichlet problem, we partition the error $\xi$ into two parts, the error $\epsilon_I$ due to the interior truncation error and the error $\epsilon$ due to the boundary truncation error. $\epsilon_I$ can be estimated by the energy method, yielding
\[
|||\epsilon_I|||_{Neu}^k \leq C_I^{Neu} h^{2p} \text{ where } C_I^{Neu} \text{ is a constant independent of } h.
\]
The boundary error equation is
\[
\epsilon_{tt} = -H^{-1} M \epsilon + h^p T^{2p,Neu,B} \tag{25}
\]
where $h^p T^{2p,Neu,B}$ is the boundary truncation error. $T^{2p,Neu,B}$ depends on the derivatives of the exact solution $U$, but not $h$. Moreover, only the first $m$ elements of $T^{2p,Neu,B}$ are nonzero, where $m$ depends on $p$ but not $h$.

We Laplace transform Equation (25), with the notation $\tilde{s} = sh$, we obtain
\[
\tilde{s}^2 \tilde{\epsilon} = -h^2 H^{-1} M \tilde{\epsilon} + h^p T^{2p,Neu,B} \tag{26}
\]
Comparing with the error equation for the Dirichlet problem (10), there are less rows affected by the boundary closure than that for the Dirichlet problem. The characteristic equations of the interior error equations are the same as for the Dirichlet problem (13). Lemma 2.2 and 2.3 are also applicable to the Neumann problem. For the error equation near the boundary, we analyze below the second, fourth and sixth order accurate cases.

3.2.1 Second order accurate scheme

For second order accurate scheme, only the first row of the error equation is affected by the boundary closure. The general solution of the error equation is
\[
\dot{\epsilon}_j = \sigma \kappa_1^j, \ j = 0, 1, 2, \cdots, \tag{27}
\]
where \( \kappa_1 = 1 - \hat{s} + \mathcal{O}(\hat{s}^2) \) is obtained from (14a) and \( \sigma \) will be determined by the boundary system. The first row of (26) is

\[
\hat{s}^2 \hat{e}_0 = -2\hat{e}_0 + 2\hat{e}_1 + h^3 \hat{T}_0^{2,\text{Neu},B}.
\]

From Equation (27), we obtain

\[
C_{2N}(\hat{s})\sigma = h^3 \hat{T}_0^{2,\text{Neu},B}, \quad C_{2N}(\hat{s}) = \hat{s}^2 + 2 - 2\kappa_1 = 2\hat{s} + \mathcal{O}(\hat{s}^2).
\]  (28)

Clearly, \( C_{2N}(0) = 0 \). By Taylor expansion, we have

\[
\hat{T}_0^{2,\text{Neu},B} = -\hat{U}_{xxx}(0, s) + \frac{1}{3} \hat{U}_{xxx}(0, s) = -\frac{2}{3} \hat{U}_{xxx}(0, s).
\]

where \(-h^3 \hat{U}_{xxx}(0, s)\) is the truncation error by the SBP approximation and \(h^3 \hat{U}_{xxx}(0, s)/3\) is the truncation error by the SAT. Therefore, we have \(|\sigma| \leq \frac{C}{|s|} |\hat{U}_{xxx}(0, s)|h^2\). In the same way as for the Dirichlet problem, an estimate in physical space follows, and we find that the boundary error is \( \mathcal{O}(h^2) \). Since the interior error is also \( \mathcal{O}(h^2) \), the convergence rate is 2. For second order accurate scheme, we gain two orders from the boundary truncation error in the Dirichlet problem, but only gain one order in the Neumann problem. Fortunately, this does not affect the overall convergence rate.

### 3.2.2 Fourth and sixth order accurate scheme

We follow the above approach to derive the four by four boundary system

\[
C_{4N}(\hat{s})\Sigma_{4N} = h^4 \hat{T}_u^{4,\text{Neu},B},
\]

for the fourth order scheme. At \( \hat{s} = 0 \) we find that \( C_{4N}(0) \) is singular with rank 3. By Taylor expansion, we derive the precise form of \( \hat{T}_u^{4,\text{Neu},B} \). To derive a sharp estimate for \( |\Sigma_{4N}| \), we write \( C_{4N}(\hat{s}) = C_{4N}(0) + \hat{s}C_{4N}'(\hat{s}) + \mathcal{O}(\hat{s}^2) \) and use Lemma 3.4 in [15]. Let singular value decomposition of \( C_{4N}(0) \) be \( U_{4N}^* S_{4N} V_{4N} \). We find that \( U_{4N}^* C_{4N}'(0) V_{4N} = -0.3095 \neq 0 \). Moreover, \( \hat{T}_u^{4,\text{Neu},B} \) is in the column space of \( C_{4N}(0) \). Hence, \( |\Sigma_{4N}| \leq K_{4N} |\hat{U}_{xxx}(0, s)|h^4 \) where \( K_{4N} \) is a constant independent of \( h \). This means that the boundary error is \( \mathcal{O}(h^4) \) and there is a gain of 2 in accuracy order. In this case, the interior error is also \( \mathcal{O}(h^4) \), and the overall convergence rate is 4. We show \( C_{4N}(0), C_{4N}'(0) \) and \( \hat{T}_u^{4,\text{Neu},B} \) in Appendix 2.

The situation of the sixth order scheme is very similar to that of the fourth order scheme. The six by six boundary system

\[
C_{6N}(\hat{s})\Sigma_{6N} = h^5 \hat{T}_u^{6,\text{Neu},B}
\]

is singular at \( \hat{s} = 0 \) with rank 5. The exact form of \( \hat{T}_u^{6,\text{Neu},B} \) is derived by Taylor expansion. Here again we find that Lemma 3.4 in [15] is applicable with \( U_{6N}^* C_{6N}'(0) V_{6N} = 0.2072 - 0.0001i \neq 0 \), and \( \hat{T}_u^{6,\text{Neu},B} \) is in the column space of \( C_{6N}(0) \). As a consequence, the boundary error is \( \mathcal{O}(h^5) \). Since the interior error is \( \mathcal{O}(h^5) \), the convergence rate is 5. \( C_{6N}(0), C_{6N}'(0) \) and \( \hat{T}_u^{6,\text{Neu},B} \) are given in Appendix 2.
Remark For fourth and sixth order scheme, the optimal $p+2$ convergence rate relies on the fact that the boundary truncation error vector is in the column space of $C_{4/6N}(0)$. In the numerical experiments in §6, we will verify the optimal convergence rate. If the boundary truncation error would not be in the column space of $C_{4/6N}(0)$, we only obtain $p+1$ convergence rate by using Lemma 3.4 in [15]. In the numerical experiments, we will add a dissipative term to the boundary part of the SBP operator, so that the boundary truncation error is not in the column space of $C_{4/6N}(0)$ but remains the same magnitude. We indeed observe $(p+1)^{th}$ order convergence rate.

4 One dimensional wave equation with a grid interface

In this section, we consider another example that does not satisfy the determinant condition. It is the Cauchy problem for the second order wave equation in one dimension

$$
U_{tt} = U_{xx} + F, \quad x \in (-\infty, \infty), \quad t \geq 0, \quad ||U(\cdot, t)|| < \infty \\
U(x, 0) = f^1(x), \quad U_t(x, 0) = f^2(x),
$$

(29)

where the forcing function $F$, the initial data $f^1$ and $f^2$ are compatible smooth functions with compact support. It is straightforward to derive the energy estimate of the form (3).

We solve the equation on a grid with a grid interface at $x = 0$. With the assumption that the exact solution is smooth, it is natural to impose two interface conditions at $x = 0$: continuity of the solution and continuity of the first derivative of the solution.

We introduce the grid on the left $x_{-j} = -jh_L$, $j = 0, 1, 2, \cdots$, and the grid on the right $x_j = jh_R$, $j = 0, 1, 2, \cdots$, with the grid size $h_L$ and $h_R$, respectively. The grid interface is denoted at $x = 0$. The grid functions are $u^L_j(t) \approx U(x_{-j}, t)$ and $u^R_j(t) \approx U(x_j, t)$. Denote

$$
e_0^L = [\cdots, 0, 0, 0]^T, \quad e_0^R = [1, 0, 0, 0, \cdots]^T, \\
u^L = [\cdots, u_{-1}^L, u_0^L]^T, \quad u^R = [u_0^R, u_1^R, \cdots]^T.
$$

Both $u_0^L = e_0^T L u^L$ and $u_0^R = e_0^T R u^R$ approximate $U(0, t)$. Both $(S_L u^L)_0 = e_0^T L S_L u^L$ and $(S_R u^R)_0 = e_0^T R S_R u^R$ approximate $U_x(0, t)$. To simplify notation, we define $\{u\} = u_0^L - u_0^R$ and $\{Su\} = (S_L u^L)_0 - (S_R u^R)_0$. The semi-discretized equation reads

$$
u^L_{tt} = D_L u^L + \frac{1}{2} H^{-1}_L S_L e_0 L \{u\} - \frac{1}{2} H^{-1}_L e_0 L \{Su\} - \tau_L H^{-1}_L e_0 L \{u\} + F_{gL}, \\
u^R_{tt} = D_R u^R + \frac{1}{2} H^{-1}_R S_R e_0 R \{u\} - \frac{1}{2} H^{-1}_R e_0 R \{Su\} - \tau_R H^{-1}_R e_0 R \{u\} + F_{gR},
$$

(30)

where $F_{gL}$ and $F_{gR}$ are the grid functions corresponding to $F(x, t)$. The penalty parameters $\tau_L$ and $\tau_R$ are chosen so that the semi-discretization is stable. By the
Take the Laplace transform in time of the interface error equation, and obtain

\[ \varepsilon_{t}^{L} = D_{L}e^{L} + \frac{1}{2}H_{L}^{-1}S_{L}^{T}e_{0L}\{\varepsilon\} - \frac{1}{2}H_{L}^{-1}e_{0L}\{S\varepsilon\} - \tau H_{L}^{-1}e_{0L}\{\varepsilon\} + h_{L}^{p}T_{2p,L,B}^{2p}, \]

\[ \varepsilon_{t}^{R} = D_{R}e^{R} + \frac{1}{2}H_{R}^{-1}S_{R}^{T}e_{0R}\{\varepsilon\} - \frac{1}{2}H_{R}^{-1}e_{0R}\{S\varepsilon\} + \tau H_{R}^{-1}e_{0R}\{\varepsilon\} + h_{R}^{p}T_{2p,R,B}^{2p}, \]

where \( h_{L}^{p}T_{2p,L,B}^{2p} \) and \( h_{R}^{p}T_{2p,R,B}^{2p} \) are the forcing terms. We take the Laplace transform in time of the interface error equation, and obtain

\[ \tilde{s}_{L}^{2}\tilde{e}_{L}^{L} = h_{L}^{2}D_{L}\tilde{e}_{L}^{L} + \frac{h_{L}^{2}}{2}H_{L}^{-1}S_{L}^{T}e_{0L}\{\varepsilon\} - \frac{h_{L}^{2}}{2}H_{L}^{-1}e_{0L}\{S\varepsilon\}, \]

\[ - \tau h_{L}^{2}H_{L}^{-1}e_{0L}\{\varepsilon\} + h_{L}^{p+2}\tilde{T}_{2p,L,B}^{2p}, \]

\[ \tilde{s}_{R}^{2}\tilde{e}_{R}^{R} = h_{R}^{2}D_{R}\tilde{e}_{R}^{R} + \frac{h_{R}^{2}}{2}H_{R}^{-1}S_{R}^{T}e_{0R}\{\varepsilon\} - \frac{h_{R}^{2}}{2}H_{R}^{-1}e_{0R}\{S\varepsilon\}, \]

\[ + \tau h_{R}^{2}H_{R}^{-1}e_{0R}\{\varepsilon\} + h_{R}^{p+2}\tilde{T}_{2p,R,B}^{2p}, \]

where \( \tilde{s}_{L} = sh_{L} \) and \( \tilde{s}_{R} = sh_{R} \). We use normal mode analysis to derive the error estimates for the second and fourth order method. The result is summarized in the following theorem.

**Theorem 4.1.** For the second and fourth order stable SBP-SAT approximation (30) of the Cauchy problem with a grid interface, the numerical solution converges to the true solution at rate \( q \). The values of \( q \) depend on \( \tau \), and are listed in Table 3.

We use the notation \( h = h_{L} = rh_{R} \) in the proof where \( r \) is the mesh size ratio. The proof follows in the same approach as before. We construct the characteristic equation on each side and solve them to obtain the general solution,

<table>
<thead>
<tr>
<th>( 2p )</th>
<th>( q(\tau &gt; \tilde{\tau}_{2p}) )</th>
<th>( q(\tau = \tilde{\tau}_{2p}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
<td>1.5</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>2.5</td>
</tr>
</tbody>
</table>

Table 3: Theoretical convergence result for one dimensional wave equation with a grid interface.
which are given by (13) and (14), respectively. The boundary system is formulated by inserting the general solution to the error equation. The accuracy order is determined by how the solution of this system behaves with respect to \( h \) in the vicinity of \( \tilde{s} = 0 \).

### 4.1 Proof of Theorem 4.1 for the second order scheme

Near the interface, the last three rows of (31) and the first three rows of (32) are affected by the penalty terms. The six by six boundary system takes the form

\[
C_{2I}(\tilde{s}, \tau) \Sigma = h^3 \hat{T}^{2,B}_u,
\]

where

\[
\Sigma = [\sigma_{1L}, \sigma_{1R}, \epsilon^L_0, \epsilon^L_{-1}, \epsilon^R_1, \epsilon^R_0]^T,
\]

\[
\hat{T}^{2,B}_u = \begin{bmatrix} 2/3 + \frac{1}{3r^2}, 0, 0, -2/3r - \frac{r}{3}, 0, 0 \end{bmatrix}^T \hat{U}_{xxx}(0,s).
\]

\( C_{2I}(0, \tau) \) is singular with rank 5 if \( \tau > \tilde{\tau}_2 \), and singular with rank 4 if \( \tau = \tilde{\tau}_2 \). The Taylor expansion of \( C_{2I}(\tilde{s}, \tau) \) at \( \tilde{s} = 0 \) is given in Appendix 3.

In the case \( \tau > \tilde{\tau}_2 \), we use the Taylor expansion of \( C_{2I}(\tilde{s}, \tau) \) at \( \tilde{s} = 0 \), and Lemma 3.4 in [15] to derive an estimate for \(|\Sigma|\). We need to perform singular value decomposition (SVD) on \( C_{2I}(0, \tau) \), which is very difficult due to the variable \( \tau \) in the matrix. Instead, we compute numerically the SVD of \( C_{2I}(0, \tau) \) for \( \tau = 1.1\tilde{\tau}_2, 1.2\tilde{\tau}_2, \ldots, 5\tilde{\tau}_2 \). In all cases, we find that \((U^tC_{2I}(0, \tau)V)_{66} \neq 0 \), and that \( \hat{T}^{2,B}_u \) is not in the column space of \( C_{2I}(0, \tau) \). Therefore, in a vicinity of \( |\tilde{s}| = 0 \), we have \( |C_{2I}^{-1}(\tilde{s}, \tau)| \leq K_c|\tilde{s}|^{-1} \). Thus,

\[
|\Sigma| \leq |C_{2I}^{-1}(\tilde{s}, \tau)||\hat{T}^{2,B}_u|h^3 \leq K_c|\tilde{s}|^{-1}|\hat{U}_{xxx}(0,s)|h^3 \leq \frac{K_c}{\eta} |\hat{U}_{xxx}(0,s)|h^2,
\]

where \( \text{Re}(\tilde{s}) \geq h\eta > 0 \) and \( K_c \) is independent of \( h \) and \( s \). For the error \( \tilde{\epsilon} \) in \( L_2 \) norm \( \|\tilde{\epsilon}\|^2_{h_L} = \|\tilde{\epsilon}^L\|^2_{h_L} + \|\tilde{\epsilon}^R\|^2_{h_R} \), we have

\[
\|\tilde{\epsilon}\|^2_{h} = h_L \sum_{i=0}^{1} |\tilde{\epsilon}^L_{-i}|^2 + h_R \sum_{i=0}^{1} |\tilde{\epsilon}^R_{i}|^2 + h_L |\sigma_L|^2 \sum_{i=0}^{\infty} |\kappa_{1L}|^{2i} + h_R |\sigma_R|^2 \sum_{i=0}^{\infty} |\kappa_{1R}|^{2i}
\]

\[
= h_L \sum_{i=0}^{1} |\tilde{\epsilon}^L_{-i}|^2 + h_R \sum_{i=0}^{1} |\tilde{\epsilon}^R_{i}|^2 + \frac{h_L |\sigma_L|^2}{1 - |\kappa_{1L}|^2} + \frac{h_R |\sigma_R|^2}{1 - |\kappa_{1R}|^2}
\]

\[
\leq \frac{K_c}{\eta^2} |\hat{U}_{xxx}(0,s)|^2 h^5 + \frac{K_c}{\eta^3} |\hat{U}_{xxx}(0,s)|^2 h^5
\]

\[
\leq \frac{K_c}{\eta^3} |\hat{U}_{xxx}(0,s)|^2 h^4.
\]

As before, we obtain

\[
\sqrt{\int_0^{t_f} \|\tilde{\epsilon}\|^2_{h} dt} \leq h^2 \sqrt{\frac{K_c}{\eta^3}} \int_0^{t_f} |U_{xxx}(0,t)|^2 dt.
\]
Thus, the interface error is $O(h^2)$ and the accuracy gain is only one order. In this case, the interior error can be estimated to $O(h^2)$ by an energy estimate, and the overall convergence rate is therefore 2.

In the case $\tau = \tilde{\tau}_2$, the numerical scheme is still stable but the above analysis is no longer valid. By the energy estimate, the convergence rate is $p + \frac{1}{2} = 1.5$.

4.2 Proof of Theorem 4.1 for the fourth order scheme

In this case, the eight by eight boundary system takes the form

$$C_{4I}(\tilde{s}, \tau)\Sigma = h^4 \hat{T}_u^{4,B},$$

where

$$\Sigma = [\sigma_{1L}, \sigma_{2L}, \sigma_{1R}, \sigma_{2R}, \epsilon_0, \epsilon_{1L}, \epsilon_{0R}, \epsilon_{1R}]^T,$$

$$\hat{T}_u^{4,B} = \begin{bmatrix}
115 & 6 & 5 & 115 & 6 & 5 & 5 & 115 \\
204 & 17r^4 & 516r^4 & 588r^4 & 204r^4 & 17r^4 & 516r^4 & 588r^4
\end{bmatrix}^T \hat{U}_{xxxx}(0, s).$$

The boundary system is also singular in this case. The Taylor expansion of $C_{4I}(\tilde{s}, \tau)$ at $\tilde{s} = 0$ is given in Appendix 3. We find that $C_{4I}(0, \tau)$ is singular with rank 7 if $\tau > \tilde{\tau}_4$, and singular with rank 6 if $\tau = \tilde{\tau}_4$.

In the case $\tau > \tilde{\tau}_4$, Lemma 3.4 in [15] is applicable since $\hat{T}_u^{4,B}$ is in the column space of $C_{4I}(0, \tau)$. We have

$$|\Sigma| \leq K_\Sigma |\hat{U}_{xxxx}(0, s)|h^4,$$

where $K_\Sigma$ is independent of $h$ and $s$. As for the second order case, it then follows that the interface error is $O(h^4)$, that is, the gain in accuracy order at the interface is 2. In this case, the interior error is $O(h^4)$ given by an energy estimate. Therefore, the convergence rate is 4.

In the case $\tau = \tilde{\tau}_4$, the numerical scheme is still stable, and the energy estimate gives a sharp estimate. The convergence rate is $p + \frac{1}{2} = 2.5$.

5 Two dimensional wave equation

In this section, we consider the second order wave equation in two dimensions:

$$U_{tt} = U_{xx} + U_{yy} + F, \ x \in [0, \infty), \ y \in (-\infty, \infty), \ t \geq 0,$$

$$U(x, y, 0) = f^1(x, y), \ U_t(x, y, 0) = f^2(x, y).$$

(33)

We consider the half plane problem in $x$ with Dirichlet boundary condition

$$U(0, y, t) = g(y, t).$$

(34)

The domain in $y$ is the whole real line. For convenience, we require that all data are $2\pi$-periodic in $y$ so that we only need to deal with a finite interval $y \in [0, 2\pi]$. In addition, we assume that the functions $F$, $f^1$, $f^2$ and $g$ are compatible smooth functions with compact support. The $L_2$ norm of the solution is bounded, i.e. $\|U\| < \infty$. Similar to the wave equation in one dimension, with homogeneous
Dirichlet boundary condition the continuous energy \( E = \| U_t \|^2 + \| U_x \|^2 + \| U_y \|^2 \) is bounded by the data.

Next, we introduce the grid and grid functions. In order to simplify notation, we assume that the mesh size is \( h \) in both \( x \) and \( y \) direction. The grid is

\[
x_i = ih, \quad i = 0, 1, 2, \ldots, \quad y_j = jh, \quad j = 0, 1, 2, \ldots, N_y,
\]
such that \( h = \frac{2\pi}{N_y} \), and the grid functions are \( u_{ij}(t) \approx U(x_i, y_j, t) \). We arrange the grid functions \( u_{ij}(t) \) column wise in a vector \( u \). The general notation used to expand an operator from one dimension to two dimensions is \( A_x = A_x \otimes I_y \), where \( \otimes \) is Kronecker product and \( I_y \) is the identity operator. With homogeneous boundary condition, the semi-discretized equation reads

\[
u_{tt} = D_{xx}u + D_{yyp}u - H^{-1}S^TE_0u - \frac{\tau}{h}H^{-1}E_0u + F_g. \tag{35}\]

\( D_{xx} \) is the standard SBP operator approximating \( \frac{\partial^2}{\partial x^2} \) and \( D_{yyp} \) is the standard central finite difference operator approximating \( \frac{\partial^2}{\partial y^2} \). In the same way as for the wave equation in one dimension, a discrete energy estimate is obtained if the penalty parameter \( \tau \) is chosen so that \( \tau \geq \frac{1}{\alpha_{2p}} \), where the values of \( \alpha_{2p} \) are listed in Table 1.

### 5.1 Accuracy analysis

We analyze the accuracy of the numerical scheme by normal mode analysis. Denote \( \epsilon \) the pointwise error due to the boundary truncation error. Then the boundary error equation is

\[
\epsilon_{tt} = D_{xx}\epsilon + D_{yyp}\epsilon - H^{-1}S^TE_0\epsilon - \frac{\tau}{h}H^{-1}E_0\epsilon + h^pT^{2p},
\]

where \( ||\epsilon||_h < \infty \). We take the Laplace transform in \( t \) and Fourier transform in \( y \), and obtain for every \( \omega \)

\[
\hat{s}^2 \hat{\epsilon}_\omega = h^2 D_{xx} \hat{\epsilon}_\omega - h^2 H^{-1}S^TE_0 \hat{\epsilon}_\omega - \tau h H^{-1}E_0 \hat{\epsilon}_\omega + h^{p+2} \hat{T}^{2p}, \tag{36}\]

where \( \hat{s} = \sqrt{\hat{s}^2 - h^2 \hat{D}_{yyp}^{\omega}} \), \( \hat{s} = sh \) and \( \hat{D}_{yyp}^{\omega} \) is the Fourier transform of \( D_{yyp} \).

For different orders of accuracy, we have

\[
\hat{D}_{yyp}^{\omega} = \begin{cases} 
-\frac{4}{\pi^2} \sin^2 \frac{\omega h}{2} & \text{if } 2p = 2, \\
-\frac{4}{\pi^2} \sin^2 \frac{\omega h}{2} \left( 1 + \frac{1}{3} \sin^2 \frac{\omega h}{2} \right) & \text{if } 2p = 4, \\
-\frac{4}{\pi^2} \sin^2 \frac{\omega h}{2} \left( 1 + \frac{1}{3} \sin^2 \frac{\omega h}{2} + \frac{8}{15} \sin^4 \frac{\omega h}{2} \right) & \text{if } 2p = 6.
\end{cases}
\]

Note that \( \hat{D}_{yyp}^{\omega} \) is nonpositive.

**Lemma 5.1.** For \( Re(\hat{s}) > 0 \) and \( \hat{D}_{yyp}^{\omega} \) defined above, it follows that \( Re(\hat{s}+) > 0 \).

**Proof.** By the definition of principal square root, \( Re(\hat{s}+) \geq 0 \). Assume \( Re(\hat{s}+) = 0 \), then \( \hat{s}^2 - h^2 \hat{D}_{yyp}^{\omega} \) is real and nonpositive, i.e. \( Re(\hat{s}^2 - h^2 \hat{D}_{yyp}^{\omega}) \leq 0 \). We then obtain \( Re(\hat{s}^2) \leq Re(h^2 \hat{D}_{yyp}^{\omega}) \leq 0 \). This contradicts \( Re(\hat{s}) > 0 \). Therefore, \( Re(\hat{s}+) > 0 \). 

\[ \square \]
The truncation error $T^{2p}$ can be written as $T^{2p} = [T_0^{2p}; T_1^{2p}; \ldots ]$, where $T_i^{2p} = [T_i^{2p}; T_{1i}^{2p}; \ldots ; T_{iN_y}^{2p}]$ is an $N_y + 1$-by-$1$ vector. For $2p^{th}$ order accurate method, we have

$$T_{kj}^{2p} = c_k U^{(p+2)}(x_k, y_j, t), \quad 0 \leq k \leq m - 1, \quad 0 \leq j \leq N_y,$$

$$T_k^{2p} = 0, \quad k \geq m.$$

to the leading order, where $m = 1, 4, 6, 8, 11$ for $2p = 2, 4, 6, 8, 10$, $c_k$ is a constant independent of $h$, $U^{(p+2)} := \frac{\partial^{p+2} U}{\partial x^{p+2}}$, and $0$ is a zero vector of size $N_y + 1$-by-$1$.

We take the Fourier transform in $y$ and Laplace transform in $t$, and obtain

$$\tilde{T}_k^{2p} = c_k \tilde{U}^{(p+2)}(x_k, \omega, s), \quad 0 \leq k \leq m - 1,$$

$$\tilde{T}_k^{2p} = 0, \quad k \geq m.$$

Similar to the one dimensional case, we only need to consider a vicinity of $|\tilde{s}| = 0$ with $\text{Re}(\tilde{s}) > 0$. By Lemma 5.1, we have $\text{Re}(\tilde{s}_+) > 0$. The boundary part of Equation (36) can be written in the matrix vector multiplication form

$$C(\tilde{s}_+, \tau) \Sigma_\omega = h^{p+2} \tilde{T}_\omega^{2p, B}.$$

We then need to investigate the invertibility of $C(\tilde{s}_+, \tau)$ and the dependence of $|C^{-1}(\tilde{s}_+, \tau) \tilde{T}_\omega^{2p}|$ on $h$. We note that Equation (36) is analogous to the error equation (10) in one dimensional case, and the matrix–valued function $C(\cdot, \tau)$ is the same with only the argument changed. Therefore, based on the normal mode analysis for the one dimensional problem in §2.3.1-2.3.3, for $2p = 2, 4, 6$ and $\tau > \tau_{2p}$ the boundary error in the Fourier and Laplace space is bounded as

$$\|\tilde{\epsilon}_\omega\|_h^2 \leq K_\omega \left| \frac{d^{p+2}}{dx^{p+2}} \tilde{U}(0, \omega, s) \right|^2 h^{2p+4},$$

where $K_\omega$ depends on $\eta$ but not $h$. Since the above estimate holds for every $\omega$, we sum them up and obtain

$$\sum_\omega \|\tilde{\epsilon}_\omega\|_h^2 \leq \sum_\omega K_\omega \left| \frac{d^{p+2}}{dx^{p+2}} \tilde{U}(0, \omega, s) \right|^2 h^{2p+4}.$$

By using the Parseval’s relation in the Fourier space, we obtain

$$\|\tilde{\epsilon}\|_h^2 \leq K_L \int_0^{2\pi} \left| \frac{d^{p+2}}{dx^{p+2}} \tilde{U}(0, y, s) \right|^2 dy h^{2p+4}.$$

We then use Parseval’s relation in the Laplace space, and obtain

$$\sqrt{\int_0^{t_f} \|\tilde{\epsilon}\|_h^2 dt} \leq h^{p+2} \sqrt{K_L e^{2\eta t_f} \int_0^{t_f} \int_0^{2\pi} \left| \frac{d^{p+2}}{dx^{p+2}} U(0, y, t) \right|^2 dy dt}.$$

For $2p = 2, 4, 6$, the boundary error is bounded in $O(h^{p+2})$. We know from the energy estimate that the interior error is bounded in $O(h^{2p})$. Therefore, we conclude that for second, fourth and sixth order methods, the convergence rates
are 2, 4 and 5 only if \( \tau > \tau_2 \). If \( \tau = \tau_2 \), the boundary system is singular. The convergence rate \( p + \frac{1}{2} \) given by the energy estimate is sharp. The numerical experiments in §6 agree with this conclusion.

The above analysis can be carried out also for the Neumann problem and the interface problem (with conforming grid interfaces) in two dimensions. Comparing with the corresponding one dimensional problem, the only difference in the error equation is that \( \tilde{s} \) is replaced by \( \tilde{s}_+ \). By Lemma 5.1 and the analysis thereafter, we conclude that the convergence result for the Neumann problem and the interface problem in two dimensions is the same as that for the corresponding one dimensional problem. For numerical experiments of these cases, we refer to [19].

It is not straightforward to generalize the above analysis to a two dimensional problem with non–periodic boundary conditions at all boundaries, or to a two dimensional problem with a non–conforming grid interface. Many numerical experiments of these cases, however, show an agreement with the convergence rate that is conjectured from the analysis of the corresponding one dimensional problem.

6 Numerical experiments

In this section, we perform numerical experiments to verify the accuracy analysis. We investigate how the accuracy of the numerical solution is affected by the large truncation error localized near the boundary and grid interface. In the analysis, we use the half line and half plane problem. However, in the numerical experiments, we use a bounded domain and impose boundary conditions on all boundaries weakly. We discretize in time using the classical fourth order Runge–Kutta method. The step size \( \Delta t \) in time is chosen so that the temporal error has a negligible impact of the spatial convergence result. The value of \( \Delta t \) is given in each numerical experiment.

The \( L^2 \) error and maximum error are computed as the norm of the difference between the exact solution \( u^{ex} \) and the numerical solution \( u^h \) according to

\[
\begin{align*}
\| u^h - u^{ex} \|_{L^2} &= \sqrt{h^d (u^h - u^{ex})^T (u^h - u^{ex})}, \\
\| u^h - u^{ex} \|_\infty &= \max |u^h - u^{ex}|,
\end{align*}
\]

where \( d \) is the dimension of the equation. The convergence rates are computed by

\[
q = \log \left( \frac{\| u^h - u^{ex} \|}{\| u^{2h} - u^{ex} \|} \right) / \log \left( \frac{1}{2} \right).
\]

6.1 One dimensional wave equation

We choose the analytical solution

\[
u = \cos(10\pi x + 1) \cos(10\pi t + 2), \quad 0 \leq x \leq 1, \quad 0 \leq t \leq 2,
\]

and use it to impose the Dirichlet boundary conditions at \( x = 0 \) and \( x = 1 \). The analytical solution and its derivatives do not vanish at the boundaries at the
The numerical method is stable if the step size restricted by the stability condition. With an error in the Laplace space is bounded in the maximum norm, which is observed as well. With an increased penalty parameter, the accuracy of the numerical solution is improved significantly, and the convergence rate min(2p, p + 2) is obtained. For second and fourth order accuracy cases, the accuracy difference between τ = 1.2τ2p and τ = 3τ2p is almost invisible. For sixth order accuracy case, one can see the small improvement in accuracy between τ = 1.2τ2p and τ = 3τ2p. The step size in time is Δt = 0.1h in all cases, except for the last two grid refinements of the sixth order scheme with τ = 3τ2p where Δt = 0.05h is used in order to observe the expected convergence behaviour. Note that these step sizes are much smaller than the step size restricted by the stability condition. With τ = 1.2τ2p, the numerical method is stable if Δt/h ≤ c, where the Courant number c = 1.3, 0.9 and 0.6 for second, fourth and sixth order method. For an increased penalty parameter τ = 3τ2p, the corresponding Courant numbers are 0.8, 0.5 and 0.4.

To test the Neumann problem, we use (37) as the analytical solution and

| Table 4: Convergence study for one dimensional wave equation with Dirichlet boundary conditions. |
|---|---|---|---|---|---|
| N | \|u^h - u^e_x\|_{L_2} | q_{L_2}/q_{\infty} | \|u^h - u^e_x\|_{L_2} | q_{L_2}/q_{\infty} | \|u^h - u^e_x\|_{L_2} | q_{L_2}/q_{\infty} |
| 51 | 1.02 | 1.60 | 1.60 | 1.10 | 1.10 | 1.10 |
| 101 | 1.58 | 2.53 | 2.53 | 2.66 | 2.66 | 2.66 |
| 201 | 3.62 | 4.27 | 4.27 | 2.56 | 2.56 | 2.56 |
| 401 | 1.99 | 7.46 | 7.46 | 2.52 | 2.52 | 2.52 |
| 801 | 7.04 | 1.31 | 1.31 | 2.50 | 2.50 | 2.50 |

| Table 5: Convergence study for one dimensional wave equation with Neumann boundary condition. |
|---|---|---|---|
| N | \|u^h - u^e_x\|_{L_2} | q_{L_2}/q_{\infty} | \|u^h - u^e_x\|_{L_2} | q_{L_2}/q_{\infty} |
| 51 | 1.84 | 1.46 | 1.46 | 9.56 | 9.56 |
| 101 | 3.76 | 3.79 | 3.79 | 1.94 | 1.94 |
| 401 | 8.93 | 9.03 | 9.03 | 8.64 | 8.64 |
| 801 | 2.97 | 1.16 | 1.16 | 1.20 | 1.20 |

final time t = 2. The L2 error, the convergence rates in L2 norm and maximum norm are shown in Table 4. The convergence rates behave as expected. With a 2p\textsuperscript{th} (2p = 2, 4, 6) order accuracy method, the convergence rate is \( p + \frac{1}{2} \) in L2 norm if the penalty parameter τ equals its limit. In this case, the pointwise error in the Laplace space is bounded in O(h\(p\)). We can hope for p\textsuperscript{th} order convergence rate in the maximum norm, which is observed as well. With an increased penalty parameter, the accuracy of the numerical solution is improved significantly, and the convergence rate min(2p, p + 2) is obtained. For second and fourth order accuracy cases, the accuracy difference between τ = 1.2τ2p and τ = 3τ2p is almost invisible. For sixth order accuracy case, one can see the small improvement in accuracy between τ = 1.2τ2p and τ = 3τ2p. The step size in time is Δt = 0.1h in all cases, except for the last two grid refinements of the sixth order scheme with τ = 3τ2p where Δt = 0.05h is used in order to observe the expected convergence behaviour. Note that these step sizes are much smaller than the step size restricted by the stability condition. With τ = 1.2τ2p, the numerical method is stable if Δt/h ≤ c, where the Courant number c = 1.3, 0.9 and 0.6 for second, fourth and sixth order method. For an increased penalty parameter τ = 3τ2p, the corresponding Courant numbers are 0.8, 0.5 and 0.4.

To test the Neumann problem, we use (37) as the analytical solution and
impose Neumann boundary condition at two boundaries \( x = 0 \) and \( x = 1 \). The \( L_2 \) error and the convergence rate in \( L_2 \) norm are shown in Table 5 in Column 2 and 3 for the fourth order scheme. Fourth order convergence rate is clearly observed, which corresponds to the optimal accuracy order gain of two from the boundary truncation error. In the accuracy analysis in §3, the optimal convergence rate relies on the fact that the truncation error vector is in the column space of \( C_{4N}(0) \). We add a dissipative term to the boundary block of the SBP operator so that the boundary truncation error vector is in the same magnitude but no longer in the column space of \( C_{4N}(0) \). The result is listed in Column 4 and 5 in Table 5. Now the gain in accuracy order is only one, and third order convergence rate is obtained as expected. Note that an energy estimate is also valid for the perturbed problem and guarantees stability. We repeat the same experiments with the sixth order scheme. The convergence rate is between five and six. We then add a dissipative term in the same way as for the fourth order scheme. The optimal accuracy order gain is lost, and the convergence rate drops to four.

Next, we test how the accuracy and convergence are affected by the large truncation error localized near a grid interface. We choose the same analytical solution (37). The grid interface is located at \( x = 0.5 \) in the computational domain \( \Omega = [0, 1] \), and the grid size ratio is 2 : 1. The step size in time is \( \Delta t = 0.1h \), where \( h \) is the smaller grid size. Note that the analytical solution does not vanish at the grid interface. We use the SAT technique to impose the outer boundary condition weakly and choose the boundary penalty parameters strictly larger than its limit. The interface conditions are also imposed by the SAT technique. We use different interface penalty parameters to see how they affect the accuracy and convergence. The results are shown in Table 6, where \( N \) denotes the number of grid points in the coarse domain.

According to the accuracy analysis in §4, for second and fourth order accu-
the analysis in maximum norm. The results from the numerical experiments agree well with much smaller. The convergence rates are $\min(2^p, p)$.

The step size in time is $\Delta t = \frac{1}{401}$. Cosine and sine are 1 and 7, respectively. However, due to the high accuracy, the error decreases clearly observed. With a larger penalty parameter, we expect the convergence to be 6 and 7, respectively. However, due to the high accuracy, the error decreases fast to the machine precision. Therefore, the expected convergence rates are not clearly observed.

### Remark

The numerical experiments with $8^{th}$ and $10^{th}$ order SBP operators are also carried out. When the penalty parameter equals its lower limit, 4.5 and 5.5 convergence rate in $L_2$ norm, and 4 and 5 convergence in maximum norm are clearly observed. With a larger penalty parameter, we expect the convergence to be 6 and 7, respectively. However, due to the high accuracy, the error decreases fast to the machine precision. Therefore, the expected convergence rates are not clearly observed.

### 6.2 Two dimensional wave equation

For two dimensional simulation, we choose the analytical solution

$$u = \cos(12x+1) \cos(4\pi y+2) \cos(\sqrt{12^2 + (4\pi)^2} t+3), \quad 0 \leq x \leq 1, \ 0 \leq y \leq 1, \ 0 \leq t \leq 2,$$

and use it to impose the Dirichlet boundary condition at $x = 0$ and $x = 1$. Periodic boundary condition is imposed at $y = 0$ and $y = 1$. The numbers of grid points are the same in $x$ and $y$ direction, and denoted by $N$ in Table 7. The step size in time is $\Delta t = 0.1h$. We clearly observe that with a $2p^{th}$ order method and $\tau = \tau_{2p}$, the convergence rates in $L_2$ norm are $p + \frac{1}{2}$ and in maximum norm are $p$. With an increased penalty parameter, the errors in $L_2$ norm are much smaller. The convergence rates are $\min(2p, p + 2)$ in both $L_2$ norm and maximum norm. The results from the numerical experiments agree well with the analysis in §5.

<table>
<thead>
<tr>
<th>$\tau = \tau_{2p}$</th>
<th>Second Order</th>
<th>Fourth Order</th>
<th>Sixth Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$|u^h - u^{ex}|_{L_2}$</td>
<td>$|u^h - u^{ex}|<em>{L</em>\infty}$</td>
<td>$|u^h - u^{ex}|_{12}$</td>
</tr>
<tr>
<td>26</td>
<td>$1.05 \times 10^{-1}$</td>
<td>$3.48 \times 10^{-2}$</td>
<td>$2.27 \times 10^{-2}$</td>
</tr>
<tr>
<td>51</td>
<td>$3.72 \times 10^{-2}$</td>
<td>$6.48 \times 10^{-3}$</td>
<td>$2.43/1.98$</td>
</tr>
<tr>
<td>101</td>
<td>$1.26 \times 10^{-3}$</td>
<td>$1.56/1.02$</td>
<td>$2.47/2.03$</td>
</tr>
<tr>
<td>201</td>
<td>$4.34 \times 10^{-3}$</td>
<td>$1.54/1.02$</td>
<td>$2.49/2.03$</td>
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<tr>
<td>401</td>
<td>$1.51 \times 10^{-3}$</td>
<td>$1.53/1.01$</td>
<td>$2.50/2.02$</td>
</tr>
</tbody>
</table>

Table 7: Convergence study for two dimensional wave equation.
7 Conclusion

For the second order wave equation a stable numerical scheme does not automatically satisfy the determinant condition. We have considered stable SBP–SAT schemes for the Dirichlet, Neumann and interface problems. In all these cases the boundary truncation error is larger than the interior truncation error. We find that only the Dirichlet problem with penalty parameter greater than its limit value satisfies the determinant condition, and in agreement with [8, 17], and a gain of two in accuracy order for the boundary error follows. Also in this case, the determinant condition is necessary for the optimal convergence rate.

For all the other cases the determinant condition is not satisfied. For most of these cases there is a gain in accuracy of order one or even two, though the energy estimate only implies a gain of order 1/2. We show that a careful analysis of the effect of the boundary truncation error yields sharp estimates. We also show that the results from analysis in one space dimension are valid in two space dimensions.

In particular we have found that to get the optimal gain in accuracy order for the Dirichlet problem and the grid interface problem, the penalty parameter should be chosen larger than its limit value given by stability analysis. However, we should not choose a very large penalty parameter since it does not decrease further the error in the solution but leads to a very small Courant number, thus an unnecessarily small step size in time.

Appendix 1

The matrix $C_{4D}(0, \tau)$ in §2.3.2 is

$$
C_{4D}(0, \tau) = \begin{bmatrix}
-3 & 3 - 4\sqrt{3} & \frac{-122 + 48\tau}{5} & 5 \\
-1 & -1 & \frac{85}{59} & 2 \\
\frac{55}{43} & \frac{85 + 12\sqrt{3}}{43} & -\frac{68}{43} & -\frac{59}{43} \\
\frac{-1}{49} & \frac{-37 + 3\sqrt{3}}{49} & \frac{17}{49} & 0
\end{bmatrix}.
$$

The first four columns of the matrix $C_{6D}(0, \tau)$ in §2.3.3 are

$$
C_{6D}(0, \tau) = \begin{bmatrix}
k(\tau) & 8.024525606 & -8.215717879 & 2.979430728 \\
1.823470407 & 2.350398187 & -1.867463026 & 0.5704778157 \\
-4.136345752 & -4.137556867 & 8.108447068 & -4.615068241 \\
0.8614698016 & 1.159078186 & -3.511693724 & 2.565973129 \\
-0.0951377428 & -0.0155610516 & 1.987601033 & -1.25102831 \\
-0.04002001476 & 0.1875223549 & -0.3471267779 & 0.1996244378
\end{bmatrix},
$$

where $k(\tau) = 3.165067038\tau - 9.382128117$, and the last two columns of the matrix $C_{6D}(0, \tau)$ in §2.3.3 are

$$
C_{6D}(0, \tau) = \begin{bmatrix}
3.368616929 + 0.0230536318i & 3.368616929 - 0.0230536318i \\
1.00246526 + 0.0469480026i & 1.00246526 - 0.0469480026i \\
-6.789853693 - 0.265966418i & -6.789853693 + 0.265966418i \\
4.592688087 + 0.1965568935i & 4.592688087 - 0.1965568935i \\
-3.188300477 - 0.2835125258i & -3.188300477 + 0.2835125258i \\
0.3280801113 + 0.1028755037i & 0.3280801113 - 0.1028755037i
\end{bmatrix}.
$$
Appendix 2

In §3.2.2, the boundary system for fourth and sixth order schemes are analyzed. We have for the fourth order scheme

\[
C'_{4N}(0) = \begin{bmatrix}
\frac{54}{17} & \frac{-59}{37} & \frac{5}{17} & \frac{11-4\sqrt{3}}{48} \\
-1 & 2 & -1 & \frac{-85+12\sqrt{3}}{48} \\
\frac{4}{43} & \frac{-59}{43} & \frac{55}{43} & \frac{-37+8\sqrt{3}}{49} \\
\frac{1}{49} & 0 & -\frac{1}{49} & \frac{-1}{49}
\end{bmatrix},
\]

and

\[
\hat{T}^{4,N_{eu,B}}_u = \begin{bmatrix}
\frac{43}{9} \\
\frac{12}{5} \\
\frac{11}{588}
\end{bmatrix} \hat{U}_{xxxxx}(0, s).
\]

For sixth order scheme, we have

\[
C_{6N}(0) = \begin{bmatrix}
\frac{3.8056512077}{1} & -\frac{4.6357425452}{1} & \frac{1.2794832344}{1} & -\frac{0.4493918968}{1} \\
\frac{-1.0534129693}{1} & \frac{2.3503981797}{1} & \frac{-1.8674630262}{1} & \frac{0.5704778157}{1} \\
\frac{0.6441780401}{1} & \frac{-4.1375568671}{1} & \frac{8.1084470675}{1} & \frac{-4.6150682405}{1} \\
\frac{-0.2133575916}{1} & \frac{1.1590781862}{1} & \frac{-3.5116937240}{1} & \frac{2.5659731293}{1} \\
\frac{0.1790783293}{1} & \frac{-0.9156510516}{1} & \frac{1.9876010325}{1} & \frac{-1.2510283103}{1} \\
\frac{-0.0400200148}{1} & \frac{0.1875223549}{1} & \frac{-0.3471267779}{1} & \frac{0.1996244378}{1}
\end{bmatrix},
\]

and

\[
C'_{6N}(0) = \begin{bmatrix}
0 & 0 & 0 & -0.2598847290 & 0 & 0 \\
0 & 0 & 0 & 0.3269055745 & 0 & 0 \\
0 & 0 & 0 & -1.7658674536 & 0 & 0 \\
0 & 0 & 0 & 1.8336101263 & 0 & 0 \\
0 & 0 & 0 & -0.693539173 & 0 & 0 \\
0 & 0 & 0 & 0.921421124 & 0 & 0
\end{bmatrix},
\]

and

\[
\hat{T}^{6,N_{eu,B}}_u = \begin{bmatrix}
-\frac{0.3287481378}{1} \\
\frac{0.2200796359}{1} \\
-\frac{0.5608447068}{1} \\
\frac{0.204406966}{1} \\
-\frac{0.1710063053}{1} \\
\frac{0.0514543047}{1}
\end{bmatrix} \hat{U}_{xxxx}(0, s).
\]

Appendix 3

In §4.1, the Taylor expansion of \(C_{2I}(\tilde{s}, \tau)\) at \(\tilde{s} = 0\) is

\[
C_{2I}(\tilde{s}, \tau) = C_{2I}(0, \tau) + \tilde{s}C'_{2I}(0, \tau) + \mathcal{O}(\tilde{s}^2),
\]
where

\[
C_{2I}(0, \tau) = \begin{bmatrix}
-1/2 & r & -1/2 + 2\tau h & 0 & 3/2 + 3r/2 - 2\tau h & -2r \\
-1 & 0 & 0 & 2 & -1 & 0 \\
1 & 0 & -1/4 & -1 & 1/4 & 0 \\
1/27 & -1/2 & 3/2 + 3r/2 - 2\tau h/3 & -2/3 & -1 + 2\tau h/3 & 0 \\
0 & -1 & 0 & 0 & 0 & 2 \\
0 & 1 & 1/4 & 0 & -1/4 & -1
\end{bmatrix},
\]

\[
C'_{2I}(0, \tau) = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1/r & 0 & 0 & 0 & 0
\end{bmatrix}.
\]

In §4.2, the Taylor expansion of \(C_{4I}(\tilde{s}, \tau)\) at \(\tilde{s} = 0\) is

\[
C_{4I}(\tilde{s}, \tau) = C_{4I}(0, \tau) + \tilde{s}C'_{4I}(0, \tau) + \mathcal{O}(\tilde{s}^2),
\]

where

\[
C_{4I}(0, \tau) = \begin{bmatrix}
-23/17 & 31 - 36\sqrt{3} & 28r & 4r(8\sqrt{3} - 5) & 48hr - 34 & 13 & 44r - 48hr + 44 & -72r \\
-1/17 & -1 & 0 & 0 & 11/17 & 2 & -12r/17 & 0 \\
52/17 & 12\sqrt{3} - 85 & 0 & 0 & -12r/17 & -50/17 & 40/17 & 0 \\
28/17 & -8\sqrt{3} + 37 & 0 & 0 & 9/17 & 0 & -8r/17 & 0 \\
0 & 0 & -23/17 & 31 - 36\sqrt{3} & 44r - 48hr + 44 & -72r/17 & 44r - 48hr - 34r & 13/17 \\
0 & 0 & 52/17 & 12\sqrt{3} - 85 & 32r/17 & 0 & -12r/17 & -50/17 \\
0 & 0 & -1/17 & -23/17 & -8\sqrt{3} + 37 & -8r/17 & 0 & 9/17 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix},
\]

\[
C'_{4I}(0, \tau) = \begin{bmatrix}
9/17 & 0 & 8/17 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.
\]

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**References**


Paper II
High order finite difference methods for the wave equation with non–conforming grid interfaces

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Abstract

We use high order finite difference methods to solve the wave equation in the second order form. The spatial discretization is performed by finite difference operators satisfying a summation–by–parts property. The focus of this work is on the numerical treatment of non–conforming grid interfaces. The interface conditions are imposed weakly by the simultaneous approximation term technique in combination with interface operators, which move the discrete solutions between the grids on the interface. In particular, we consider interpolation operators and projection operators. A norm–compatibility condition, which leads to stability for first order hyperbolic systems, does not suffice for second order wave equations. An extra constraint on the interface operators must be satisfied to derive an energy estimate for stability. We carry out eigenvalue analyses to investigate the additional constraint and how it is related to stability, and find that the projection operators have better stability properties than the interpolation operators. In addition, a truncation error analysis is performed to study the convergence property of the numerical schemes. In the numerical experiments, the stability and accuracy properties of the numerical schemes are further explored, and the practical usefulness of non–conforming grid interfaces is presented and discussed in two efficiency studies.

Keywords: Second order wave equation, Finite difference method, SBP–SAT, Non–conforming grid interface, Interpolation, Coupling AMS subject classifications: 65M06, 65M12, 65M15

1 Introduction

For wave propagation problems, the computational domain is often large compared with the wavelength, and waves travel for a long time. It has been shown that high order accurate discretizations in time and space are more efficient to solve these problems on smooth domains [7, 11]. Although it is straightforward to derive high order finite difference schemes in the interior of the computational

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domain, it is challenging to derive the boundary closures in a stable and accurate way. For long time simulations, it is also desirable that the discretization is strictly stable [8, pp. 129]. A successful candidate of high order finite differences is the summation–by–parts simultaneously approximation term (SBP–SAT) method [3, 26]. An SBP operator [13] approximates a spatial derivative, and mimics integration–by–parts via its associated norm. The SAT method [2] is used to impose boundary conditions and grid interface conditions weakly.

Traditionally, the wave equation is written as a first order hyperbolic system, and is then solved by the well–developed methods for such systems. However, there are various drawbacks in doing so [12]. Therefore, it is desirable to solve directly the wave equation in the second order form. In [27], an SBP–SAT method for the wave equation in the second order form is developed and the numerical treatment of conforming grid interfaces is discussed. Stability of the numerical scheme is proved by the energy method, and the convergence property is investigated in the numerical experiments.

For a wave that travels in an inhomogeneous medium, the wave speed varies in space. Since the wavelength is proportional to the wave speed, a reduction in the wave speed confined to a subset of the physical domain yields a wave with a shorter wavelength localized in that subset. In [11], the accuracy of a numerical solution to a Cauchy problem is stated in terms of the number of grid points per wavelength. For computational efficiency it is important that a fine mesh is used in the subset that constitutes the slower media, and a coarse mesh elsewhere.

To achieve this, one approach is to partition the computational domain into blocks, where the mesh sizes are constant in each block but differ in different blocks. In more than one space dimension, the partition results in non–conforming grid interfaces with hanging nodes. Suitable interface conditions are then imposed to couple adjacent mesh blocks and yield a well–posed problem. Many techniques for the numerical treatment of interface conditions have been proposed. In [24], an energy conserving discretization of the elastic wave equation in the second order formulation is presented. The finite difference operators satisfy the principle of SBP, and the grid interface with a 1:2 refinement ratio is handled by ghost points. Stability is proved by the energy method, but the convergence rate of the numerical scheme is limited to two.

In [16] the norm–compatible interpolation operators are constructed to handle non–conforming grid interfaces, and the Euler equations are used as the model problem. The norm–compatibility condition leads to an energy estimate for first order hyperbolic systems and the Schrödinger equation [22]. The interpolation error is of the same magnitude as the error due to the derivative approximations by the SBP operators. In the numerical experiments, it is shown that the convergence rate of the numerical scheme applied to the Euler equations is not lowered by using the interpolation operators, compared with the case with only conforming grid interfaces. To use the interpolation operators presented in [16], the mesh refinement ratio is fixed to 1 : 2 and the mesh blocks must be conforming.

Recently, a general purpose methodology for coupling mesh blocks with non–conforming interfaces was developed in [10]. This technique uses projection
operators to move a discrete finite difference solution to piecewise polynomial functions in a subspace of a Hilbert space where the coupling is done. The wave equation in the first order system formulation is used as the model problem. Stability is proved by the energy method, and the numerical experiments demonstrate that the convergence rate is the same as if conforming grid interfaces were used. The projection operators allow for a very flexible configuration of meshing in the sense that the interfaces as well as the mesh blocks do not need to be conforming. Similarly to the interpolation operators, the projection operators satisfy norm–compatibility conditions that are essential for the stability proof to hold.

In this paper, we focus on the numerical treatment of non–conforming grid interfaces for the wave equation in the second order form in the framework of the SBP–SAT methodology. In particular, the stability and accuracy properties are investigated. We have found that in contrast to first order hyperbolic systems for which the norm–compatibility condition leads to stability, an extra condition on the interface operator is needed to derive an energy estimate for the second order wave equation. This condition is satisfied for the second and fourth order accurate interpolation operators constructed in [14] and the projection operators in [10]. We prove stability by the energy method for those cases. For higher order accurate schemes the extra condition is not satisfied, and we cannot prove stability. With an eigenvalue analysis, we have found that the violation of the stability condition is very weak for the projection operators, and in all the numerical experiments we have conducted no unphysical growth is observed for the schemes with the projection operators. In certain cases the SBP–SAT schemes with the sixth and eighth order accurate interpolation operators are not stable.

Local mesh refinement reduces the number of grid points significantly in computations. To achieve full efficiency, the numerical scheme must also be accurate enough. It is desirable that the convergence rate is not depressed by using non–conforming grid interfaces. Even though this is in most cases true for first order hyperbolic systems, the situation for second order equations is less favourable. By a truncation error analysis, we show that the truncation error near the edge of the non–conforming grid interfaces is two orders larger than that with conforming grid interfaces. The large truncation error is only localized at a few grid points in a two dimensional space, and its effect to the convergence rate may be weakened. In fact, the numerical experiments show that the convergence rate with a non–conforming grid interface is only one order lower than the corresponding case with a conforming grid interface. In addition, an efficiency study is carried out by a comparison of the numerical schemes with interpolation operators and projection operators. We have found that in certain cases it is beneficial to use non–conforming grid interfaces, albeit the accuracy reduction.

The structure of this paper is as follows. In §2, the SBP–SAT methodology is introduced. We then discuss stability and accuracy properties of the numerical coupling based on interpolation operators in §3, and projection operators in §4. Numerical experiments are carried out in §5 including the eigenvalue analyses for stability, convergence verifications for accuracy and studies on computational
efficiency. We conclude and mention future work in §6.

2 Preliminaries

We begin with the preliminaries that will be used in the discussion of the SBP–SAT method. Let \( w_1(x) \) and \( w_2(x) \) be two real–valued functions in \( L^2[0,1] \). The inner product is defined by \( (w_1, w_2) = \int_0^1 w_1 w_2 dx \). The corresponding norm is \( \|w_1\|^2 = (w_1, w_1) \). The computational domain \([0,1]\) is discretized by \( N+1 \) equidistant grid points

\[ x_i = ih, \quad i = 0, 1, \ldots, N, \text{ where } h = \frac{1}{N}. \]

With any fixed \( N \), a grid function can be represented by a vector and an operator can be represented by a matrix. Throughout this paper, we use an operator and a matrix interchangeably when there is no ambiguity.

2.1 The SBP operators

We need the following definitions:

**Definition 2.1** A difference operator \( D_1 = H^{-1}Q \) approximating first derivative \( \partial/\partial x \) is a narrow diagonal first derivative SBP operator, if \( H \) is diagonal and positive definite, \( Q + QT = B = \text{diag}(-1, 0, \ldots, 0, 1) \) and the interior stencil width of \( D_1 \) is minimal.

**Definition 2.2** A difference operator \( D_2^{(b)} = H^{-1}(-M^{(b)} + B^{(b)}S) \) approximating second derivative \( \partial/\partial x (b(x)\partial/\partial x) \) with \( b(x) > 0 \) is a narrow diagonal variable coefficient second derivative SBP operator, if \( H \) is diagonal and positive definite, \( M^{(b)} \) is symmetric positive semidefinite, \( B^{(b)} = \text{diag}(-b(x_0), 0, \ldots, 0, b(x_N)) \), the first and last row of \( S \) is a one sided approximation of \( \partial/\partial x \) at the boundary and the interior stencil width of \( D_2^{(b)} \) is minimal.

The diagonal positive definite matrix \( H \) defines the SBP norm, and it has the interior weight \( h \) and special boundary weights. To solve the wave equation on a curvilinear grid, even if the original equation has only constant coefficients, the transformed equation has second derivative terms with variable coefficients, and mixed derivative terms. Therefore, it is important that \( D_1 \) and \( D_2^{(b)} \) are based on the same norm \( H \). In addition, \( D_1 \) and \( D_2^{(b)} \) must be compatible for the energy method to be applicable for proving stability. Compatibility [20] means that \( M^{(b)} \) can be written as \( M^{(b)} = D_1^T H B^{(b)} D_1 + R^{(b)} \) where \( R^{(b)} \) is symmetric positive semidefinite. In this case, \( D_2^{(b)} \) is essentially equal to applying \( D_1 \) twice plus a small dissipative term.

The accuracy of the SBP operators are often termed as \( 2p \), meaning that the approximation error of \( D_1 \) and \( D_2^{(b)} \) is \( \mathcal{O}(h^{2p}) \) in the interior, while near the boundary the approximation error increases to \( \mathcal{O}(h^p) \). For \( S \approx \frac{d}{dx} \) at the boundary, the approximation error is \( \mathcal{O}(h^{p+1}) \). 2\( p \)th order accurate SBP operators \( D_1 \) are constructed in [25] for \( p = 1, 2, 3, 4 \), and in [15] for \( p = 5 \). In [14],
Table 1: $\alpha_{2p}$ values

<table>
<thead>
<tr>
<th>2p</th>
<th>2</th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_{2p}$</td>
<td>0.4</td>
<td>0.2508560249</td>
<td>0.1878715026</td>
<td>0.0015782259</td>
<td>0.0351202265</td>
</tr>
</tbody>
</table>

$2p^{th}$ order accurate $D_2^{(b)}$ are constructed for $p = 1, 2, 3$, and they are compatible with $D_1$ constructed in [25]. The construction of $D_2^{(b)}$ requires to solve a large system of nonlinear equations, which makes it very involved when the accuracy order is high. In certain cases, we only need an SBP operator $D_2$ that approximates second derivative $\partial^2 / \partial x^2$, and these operators are constructed in [19] for $p = 1, 2, 3, 4$ and in [15] for $p = 5$.

The following lemma, which is often referred to as the borrowing trick [17], describes an important property of the SBP operator $D_2$ constructed in [15, 19]:

**Lemma 2.3** The matrix $M$ in $D_2$ constructed in [19] can be written as

$$M = h\alpha_{2p}(BS)^T BS + \tilde{M},$$

where $\tilde{M}$ is symmetric positive semidefinite and $\alpha_{2p}$ is a constant independent of $h$. The values of $\alpha_{2p}$ are listed in Table 1 for different accuracy orders.

A similar lemma for $D_2^{(b)}$ constructed in [14] is presented in [27].

There are other types of SBP operators as well. It is possible to increase the accuracy by using a block norm $H$, meaning that $H$ is diagonal in the interior and has a symmetric–block–structured boundary closure. In this case, the approximation error in the interior and near the boundary are $O(h^{2p})$ and $O(h^{2p-1})$, respectively. The drawback of the block norm SBP operators is that the energy method is not applicable to prove stability for the wave equation with variable coefficients and/or solved on a curvilinear grid, and unphysical growth is indeed observed in numerical experiments. This has limited the practical usage of the block norm SBP operators. In [15], artificial dissipation is added to stabilize the scheme.

### 3 Non–conforming grid interfaces handled by interpolation operators

The numerical coupling of conforming grid interfaces by the SAT method for the wave equation is discussed in [27]. Our aim in this section is to generalize the scheme to also couple non–conforming grid interfaces by using the interpolation operators constructed in [16]. To begin with, we consider the two–block–structured mesh $\Omega$ shown in Figure 1a: a coarse mesh $\Omega_L$ in the left block with $n_{xL} \times n_{yL}$ grid points and a fine mesh $\Omega_R$ in the right block with $n_{xR} \times n_{yR}$ grid points. The equality $n_{yR} = 2n_{yL} - 1$ yields a 1:2 mesh refinement ratio across the interface.

In [16], the interpolation operators are denoted by $I_{F2C}$ and $I_{C2F}$, where the subscripts $F2C$ and $C2F$ refer to fine to coarse and coarse to fine, respectively.
Though only interpolation operators for the grid interface with mesh refinement ratio 1:2 are reported, the construction of the interpolation operators with some other refinement ratios (1:4, 1:8, \cdots) is possible by the same technique. To handle a multi–block–structured mesh shown in Figure 1b, even though the interface between the left–up block and the left–down block is conforming, it is necessary to treat it as an interface to make the energy method applicable to prove stability. In other words, the mesh blocks must be conforming.

It is important that the interpolation operators preserve the SBP property. To this end, the following norm–compatibility condition is essential:

\[ H_yR I_C 2F = (H_yL I_F 2C)^T, \]  

(1)

where \( H_yL \) and \( H_yR \) are SBP norms in the left block and right block, both in the \( y \) direction.

The interpolation operators do not interpolate exactly, instead they mimic the accuracy properties of the diagonal norm SBP operators. The interpolation error is \( O(h^{2p}) \) in the interior of the interface and \( O(h^p) \) near the edge of the interface. We call them 2\( p \)th order accurate interpolation operators, and when used together with the 2\( p \)th order accurate SBP operators the scheme is also termed as 2\( p \)th order accurate, though the truncation error of the semidiscretized equation may not be \( O(h^{2p}) \) or \( O(h^p) \). Here, \( h \) is used to denote the magnitude of the mesh sizes for the sake of a simplified notation, though at most four different mesh sizes could be present in the mesh \( \Omega \).

With the above accuracy requirement and the norm–compatibility condition (1), 2\( p \)th order accurate interpolation operators are constructed for \( p = 1, 2, 3 \) and 4 in [16]. Though the accuracy is reduced near the edge of the interface, the number of grid points with the large interpolation error \( O(h^p) \) is independent of \( h \).

As will be seen later, when the interpolation operators are used to solve the wave equation an extra condition is posed on the interpolation operators in order to apply the energy method to prove stability:

\[ \Xi_L := H_yL(I_{yL} - I_{F2C}I_{C2F}) \geq 0, \quad \Xi_R := H_yR(I_{yR} - I_{C2F}I_{F2C}) \geq 0, \]  

(2)

where \( \Xi \geq 0 \) means that the matrix \( \Xi \) is symmetric positive semidefinite, and \( I_{yL}, I_{yR} \) are identity matrices. It is straightforward to show that \( \Xi_L \) and \( \Xi_R \)
are symmetric, but the positive semidefiniteness is not a built-in constraint in the construction process of the interpolation operators in [16]. In §5, an eigenvalue analysis is performed to show that (2) is satisfied for the second and fourth order accurate interpolation operators. Negative eigenvalues are present with the sixth and eighth order accurate interpolation operators. However, the scheme with sixth other accurate interpolation operators seems stable in some of the numerical experiments conducted in §5, indicating that (2) is a sufficient but not necessary condition for stability.

3.1 The wave equation with a non-conforming grid interface

The wave equation in the second order form in two space dimensions is

\[ U_{tt} = U_{xx} + U_{yy}, \]

where \(-\infty < x < \infty\), \(0 \leq y \leq 1\) and \(0 \leq t \leq t_f\). We assume that the initial conditions and boundary conditions are compatible smooth functions with compact support. As a consequence, the true solution \(U\) is also smooth. To solve the equation on the mesh \(\Omega\) shown in Figure 1a, continuity of the solution and continuity of first normal derivative across the grid interface are required.

In the numerical coupling scheme, we frequently pick up solutions along the interface by using the matrices defined in the first column of Table 2. In each of those matrices, all elements are zero except one element that is equal to one. The sizes along with the positions of the nonzero element are listed in the second and third column of Table 2. Note that \(E_{LR} = E_{RL}^T\).

Bold letters are used to denote the operators in two space dimensions, which are obtained from the corresponding one dimensional operators through the Kronecker product \(A_x = A_x \otimes I_y\) and \(A_y = I_x \otimes A_y\), where \(I_x\) and \(I_y\) are identity matrices.

Next, Equation (3) is discretized by the SBP operators on \(\Omega\) and the grid interface conditions are imposed weakly by the SAT method and interpolation operators. The semidiscretized equation corresponding to (3) reads:

\[
\begin{align*}
    u_{tt} &= D_{2L}u + SAT_{u1} + SAT_{u2} + SAT_{\partial u}, \\
    v_{tt} &= D_{2R}v + SAT_{v1} + SAT_{v2} + SAT_{\partial v},
\end{align*}
\]

Table 2: Matrices that are used to pick up solutions on the interface.

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Size</th>
<th>Nonzero</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E_{0L})</td>
<td>(n_x L \times n_x L)</td>
<td>((n_x L, n_x L))</td>
</tr>
<tr>
<td>(E_{0R})</td>
<td>(n_x R \times n_x R)</td>
<td>((1, 1))</td>
</tr>
<tr>
<td>(E_{LR})</td>
<td>(n_x L \times n_x R)</td>
<td>((n_x L, 1))</td>
</tr>
<tr>
<td>(E_{RL})</td>
<td>(n_x R \times n_x L)</td>
<td>((1, n_x R))</td>
</tr>
</tbody>
</table>
where

\[
\begin{align*}
SAT_{u1} &= \frac{1}{2} H_{xL}^{-1} S_{xL}^T (E_0 L u - (E_{LR} \otimes I_{F2C}) v), \\
SAT_{u2} &= -\tau H_{xL}^{-1} (E_0 L u - (E_{LR} \otimes I_{F2C}) v), \\
SAT_{\partial u} &= -\frac{1}{2} H_{xL}^{-1} (E_0 L S_{xL} u - (E_{LR} \otimes I_{F2C}) S_{xR} v),
\end{align*}
\]

and

\[
\begin{align*}
SAT_{v1} &= -\frac{1}{2} H_{xR}^{-1} S_{xR}^T (E_0 R v - (E_{RL} \otimes I_{C2F}) u), \\
SAT_{v2} &= -\tau H_{xR}^{-1} (E_0 R v - (E_{RL} \otimes I_{C2F}) u), \\
SAT_{\partial v} &= \frac{1}{2} H_{xR}^{-1} (E_0 R S_{xR} v - (E_{RL} \otimes I_{C2F}) S_{xL} u).
\end{align*}
\]

Here, \( u \) and \( v \) are grid functions in \( \Omega_L \) and \( \Omega_R \), respectively. \( D_{2L} \) and \( D_{2R} \) are SBP operators approximating second derivatives. In (4) the penalty terms for the boundary conditions are omitted as the focus here is the numerical treatment of the grid interface. Both \( SAT_{u1} \) and \( SAT_{u2} \) impose weakly the continuity of the solution across the grid interface. The term \( S_{xL}^T \) in \( SAT_{u1} \) makes the semidiscretization symmetric with respect to the SBP norms. The penalty parameter \( \tau \) in \( SAT_{u2} \) controls the strength of the weak enforcement, and its value is determined by the energy method. The penalty term \( SAT_{\partial u} \) imposes weakly the continuity of the first normal derivative across the grid interface. The penalty terms in Equation (4b) are constructed in a similar way.

In the following, the stability of (4) is proved by the energy method.

### 3.1.1 Stability analysis by the energy method

Multiplying Equation (4a) by \( u_t^T H_L \) and Equation (4b) by \( v_t^T H_R \), and using the equality \( E_{LR} = E_{RL}^T \) and relation (1),

\[
\begin{align*}
\frac{d}{dt} (u_t^T H_L u_t + v_t^T H_R v_t) \\
= \frac{d}{dt} (u^T (M_{xL} \otimes H_{yL}) u + u^T (E_0 L S_{xL} \otimes H_{yL}) u - \tau u^T (E_0 L \otimes H_{yL}) u \\
- v^T (M_{xR} \otimes H_{yR}) v - v^T (E_0 R S_{xR} \otimes H_{yR}) v - \tau v^T (E_0 R \otimes H_{yR}) v \\
- u^T (S_{xL}^T E_{LR} \otimes H_{yL} I_{F2C}) v + v^T (S_{xR}^T E_{RL} \otimes H_{yR} I_{C2F}) u \\
+ 2\tau u^T (E_{LR} \otimes H_{yL} I_{F2C}) v).
\end{align*}
\]

Next, the following equality is obtained by moving all terms on the right hand side of (5) to the left

\[
\frac{d}{dt} E_{H}^W = 0,
\]
where

\[ E_H^W = u_t^T H_L u_t + v_t^T H_R v_t \]
\[ + u^T (M_{xL} \otimes H_{yL}) u - u^T (E_{0L} S_{xL} \otimes H_{yL}) u + \tau u^T (E_{0L} \otimes H_{yL}) u \]
\[ + v^T (M_{xR} \otimes H_{yR}) v + v^T (E_{0R} S_{xR} \otimes H_{yR}) v + \tau v^T (E_{0R} \otimes H_{yR}) v \] \tag{7}
\[ + u^T (S_{xL}^T E_{LR} \otimes H_{yL} I_{F2C}) v - v^T (S_{xR}^T E_{RL} \otimes H_{yR} I_{C2F}) u \]
\[ - 2\tau u^T (E_{LR} \otimes H_{yL} I_{F2C}) v. \]

Then, an energy estimate exists if \( E_H^W \geq 0 \) for any \( u \) and \( v \), and in this case \( E_H^W \) is a discrete energy of the semidiscretized equation (4). To achieve this, we need relation (2) to obtain

\[ u^T (E_{0L} \otimes H_{yL}) u \geq u^T (E_{0L} \otimes H_{yL} I_{F2C} I_{C2F}) u \]
\[ = u^T (E_{0L} \otimes I_{C2F} H_{yR} I_{C2F}) u \]
\[ = ((E_{0L} \otimes I_{C2F}) u)^T (I_{xL} \otimes H_{yR}) ((E_{0L} \otimes I_{C2F}) u). \]

It then follows for \( u \):

\[ u^T (E_{0L} \otimes H_{yL}) u \geq \frac{1}{2} u^T (E_{0L} \otimes H_{yL}) u + \frac{1}{2} ((E_{0L} \otimes I_{C2F}) u)^T (I_{xL} \otimes H_{yR}) ((E_{0L} \otimes I_{C2F}) u), \] \tag{8}

and for \( v \):

\[ v^T (E_{0R} \otimes H_{yR}) v \geq \frac{1}{2} v^T (E_{0R} \otimes H_{yR}) v + \frac{1}{2} ((E_{0R} \otimes I_{F2C}) v)^T (I_{xR} \otimes H_{yL}) ((E_{0R} \otimes I_{F2C}) v). \] \tag{9}

In addition, Lemma 2.3 gives:

\[ M_{xL} = \tilde{M}_{xL} + h_{xL} \alpha_2 p (E_{0L} S_{xL})^T (E_{0L} S_{xL}), \]
\[ M_{xR} = \tilde{M}_{xR} + h_{xR} \alpha_2 p (E_{0R} S_{xR})^T (E_{0R} S_{xR}), \] \tag{10}

where \( \tilde{M}_{xL} \) and \( \tilde{M}_{xR} \) are symmetric positive semidefinite matrices.

Next, we plug in (2.3), (8) and (9) to (7), and obtain

\[ E_H^W = Q_1 + Q_2 + Q_3, \]

where

\[ Q_1 = u_t^T H_L u_t + v_t^T H_R v_t + u^T (\tilde{M}_{xL} \otimes H_{yL}) u + v^T (\tilde{M}_{xR} \otimes H_{yR}) v, \]
\[ Q_2 = h_{xL} \alpha_2 p (E_{0L} S_{xL})^T (I_{xL} \otimes H_{yL}) (E_{0L} S_{xL}) u \]
\[ - (E_{0L} S_{xL} u)^T (I_{xL} \otimes H_{yL}) (u - (E_{LR} \otimes I_{F2C}) v) \]
\[ + \frac{\tau}{2} (u - (E_{LR} \otimes I_{F2C}) v)^T (I_{xL} \otimes H_{yL}) (u - (E_{LR} \otimes I_{F2C}) v), \]
\[ Q_3 = h_{xR} \alpha_2 p (E_{0R} S_{xR} v)^T (I_{xR} \otimes H_{yR}) (E_{0R} S_{xR} v) \]
\[ - (E_{0R} S_{xR} v)^T (I_{xR} \otimes H_{yR}) ((E_{RL} \otimes I_{C2F}) u - v) \]
\[ + \frac{\tau}{2} ((E_{RL} \otimes I_{C2F}) u - v)^T (I_{xR} \otimes H_{yR}) ((E_{RL} \otimes I_{C2F}) u - v). \]
Since $\tilde{M}_xL$ and $\tilde{M}_xR$ are positive semidefinite, we have $Q_1 \geq 0$. To ensure $Q_2 \geq 0$ and $Q_3 \geq 0$, we need
\[
2\sqrt{h_{xL}\alpha_{2p}}\sqrt{\tau/2} \geq 1 \text{ and } 2\sqrt{h_{xR}\alpha_{2p}}\sqrt{\tau/2} \geq 1.
\]
\[
\Rightarrow \quad \tau \geq \max \left( \frac{1}{2\alpha_{2p}h_{xL}}, \frac{1}{2\alpha_{2p}h_{xR}} \right).
\]
In the mesh shown in Figure 1a, the mesh refinement ratio across the grid interface is $1 : 2$, i.e. $h_{xR} = \frac{1}{2}h_{xL}$. Thus,
\[
\tau \geq \frac{1}{\alpha_{2p}h_{xL}}
\]
is the condition for $E_W^W$ to be a discrete energy. Therefore, an energy estimate is obtained if (1), (2) and (11) hold.

As shown above, in order to apply the energy method (2) must be satisfied, which means that the energy estimate is only valid for the second and fourth order accurate schemes. The same interpolation operators are used for the Schrödinger equation in [22] but (2) is not needed for stability. For the Euler equations, (2) is not needed when the standard SBP operators are used for the discretization, but needed when upwind SBP operators are used [16].

### 3.1.2 Convergence rate

We discuss the accuracy properties of (4) by analyzing the truncation error of (4a). Equation (4b) can be analyzed in a similar way. The approximation error of the SBP operator $D_{2L}$ is $O(h^{2p})$ in the interior and $O(h^p)$ near the interface, with the latter one being the dominant source of error. In the first penalty term $SAT_{u1}$, a large interpolation error $O(h^p)$ is located near the edge of the grid interface. Due to the $h^{-1}$ factor in both $H^{-1}_x$ and $S^T_{xL}$, the localized truncation error of $SAT_{u1}$ is $O(h^{p-2})$. Similarly, we find that the localized truncation errors of $SAT_{u2}$ and $SAT_{\partial u}$ are $O(h^{p-2})$ and $O(h^{p-1})$, respectively. Therefore, the localized truncation error of the semidiscretization (4a) is $O(h^{p-2})$.

In [28], the convergence of the SBP–SAT discretization of the second order wave equation in one space dimension with a grid interface is analyzed. The result is that if the penalty parameter is chosen strictly larger than the limit value required for stability, the localized truncation error $O(h^p)$ near the grid interface results in an error $O(h^{p+1})$ in the solution for $p = 1$, and an error $O(h^{p+2})$ for $p \geq 2$. In other words, we gain one order in convergence if $p = 1$ and two orders if $p \geq 2$.

In our case, the spatial dimension is two and there is the possibility of another gain in convergence. That is, the number of grid points with truncation error $O(h^{p-2})$ is finite and independent of $h$. Hence, the $L_2$ norm of this truncation error is $O(h^{p-1})$, and is one order higher than the pointwise truncation error. Therefore, we can hope to get an extra gain in convergence comparing with the corresponding one dimensional case.

By a convergence test in §5, we find that the extra gain is one order, which gives a total gain of two orders for $p = 1$ and three orders for $p \geq 2$. That is,
the localized truncation error $O(h^{p-2})$ results in an error $O(h^p)$ in the solution for $p = 1$, and an error $O(h^{p+1})$ for $p \geq 2$. To obtain this convergence rate, it is important to choose the penalty parameter strictly larger than the value required for stability.

Comparing with the case of conforming grid interfaces, the convergence rate is one order lower. Even though a non–conforming grid interface allows for a local mesh refinement, the loss of accuracy may attenuate its efficiency in practice. To overcome the accuracy reduction by the non–conforming grid interfaces, we have tried to build interpolation operators with error $O(h^{2p})$ in the interior and error $O(h^{p+1})$ near the edge of the interface, based on both diagonal and block norm SBP operators by using the symbolic software MAPLE and the approach presented in [16]. However, we could not find a solution to the resulting system of equations.

### 3.2 An extension to T–junction interfaces

In Figure 1b, the interface between the two blocks on the left is conforming. It is then in many cases desirable not to consider it as a grid interface, but to use the mesh shown in Figure 2a instead, where the interface there forms a T–junction. This is because SBP operators have a larger approximation error near the grid interface than that in the interior. The usage of redundant grid interfaces results in additional errors in the solution. Moreover, avoiding T–junction interfaces may end up in a bad partitioning of the computational domain with many unnecessary mesh blocks. With a straightforward application of the interpolation operators, instability occurs around the T–junction interface intersection point. The reason is that near the interface intersection point in Figure 2a, the SBP norm in the vertical direction has the interior weights in the left domain, and the boundary weights in the two domains on the right. As a consequence, the norm–compatibility condition is violated and no energy estimate can be derived.

In [21], the T–junction operators are constructed to handle T–junction interfaces and are applied to the advection equation and the Schrödinger equation in the SBP–SAT framework. Stability is proved by the energy method, but it comes with the cost that the T–junction operators introduce an error $O(h^{2p})$ in the interior of the interface and $O(h^p)$ near the edge of the interface. The

![Figure 2: T–junction interfaces](image-url)
T–junction operators can also be used together with the interpolation operators to handle non–conforming grid interfaces. One constraint for the T–junction operators is that the interface intersection point must be a grid point in all involved mesh blocks, for example a close-up T–junction interface in Figure 2b. It is not straightforward to handle the T–junction interface shown in Figure 2c by the same technique.

4 Non–conforming grid interfaces handled by projection operators

In [10], a new methodology of handling grid interfaces is introduced. In contrast to the interpolation operators which are based on a direct interpolation technique, the new methodology is based on a projection method. The highlights are that there is no strict requirement on the mesh refinement ratio, and the mesh blocks do not need to be conforming.

To illustrate how the projection method works, we consider again the mesh Ω shown in Figure 1a, and denote \( y^L \) in \( Ω_L \) and \( y^R \) in \( Ω_R \) the grids on the interface. In addition, \( z^L \) and \( z^R \) denote the discrete finite difference solutions on \( y^L \) and \( y^R \). In a general setting, eight projection operators are used to move \( z^L \) and \( z^R \) between the two grids on the interface. Firstly, the discrete finite difference solution \( z^L \) is projected by a projection operator \( P^L_{f2p} \) to a piecewise continuous function based on the grid \( y^L \). The associated mass matrix \( M^L \) on \( y^L \) is diagonal positive definite since Jacobi polynomials are used as the basis functions. Next, the glue grid \( y \) with the mass matrix \( M^g \) is defined as the grid that consists of the grid points on both \( y^L \) and \( y^R \). The projection operator \( P^L_{p2g} \) is used to project the piecewise continuous function from \( y^L \) to \( y \), and is viewed as a basis transformation between polynomial spaces. Similarly, \( P^L_{p2f} \) and \( P^L_{g2p} \) are projection operators in the reversed direction corresponding to \( P^R_{f2p} \) and \( P^R_{p2g} \), respectively. \( P^R_{f2p}, P^R_{p2f}, P^R_{p2g} \) and \( P^R_{g2p} \) are the corresponding projection operators for the grid \( y^R \).

Similar to the interpolation operators, there are norm–compatibility conditions for the projection operators:

\[
H_{yL}P^L_{p2f} = (M^L P^L_{f2p})^T, \quad H_{yR}P^R_{p2f} = (M^R P^R_{f2p})^T, \quad \tag{12}
\]

and

\[
M^g P^L_{p2g} = (M^L P^L_{g2p})^T, \quad M^g P^R_{p2f} = (M^R P^R_{g2p})^T. \quad \tag{13}
\]

Define

\[
I^p_{L2R} = P^R_{p2f} P^R_{g2p} P^L_{p2g} P^L_{f2p} \quad \text{and} \quad I^p_{R2L} = P^L_{p2f} P^L_{p2g} P^R_{g2p} P^R_{f2p}, \quad \tag{14}
\]

the operator \( I^p_{L2R} \) moves \( z^L \) from \( y^L \) to \( y^R \), and \( I^p_{R2L} \) moves \( z^R \) from \( y^R \) to \( y^L \).

For the projection operators \( P^L_{f2p} \) and \( P^L_{p2f} \) which move the discrete finite difference solution to the subspace of piecewise continuous functions and back, the projection error is \( O(h^{2p}) \) in the interior and \( O(h^p) \) near the edge, where \( p = 1, 2, 3, 4, 5 \). \( P^{L/R}_{p2g} \) and \( P^{L/R}_{g2p} \) can be viewed as basis transformation operators between grids. As a consequence, the projection error of \( I^p_{L2R} \) and \( I^p_{L2R} \) is also
\(\mathcal{O}(h^{2p})\) in the interior and \(\mathcal{O}(h^p)\) near the edge, where \(p = 1, 2, 3, 4, 5\). In other words, \(I_{L2R}^p\) and \(I_{L2R}^p\) have the same accuracy properties as the diagonal norm SBP operators and the interpolation operators in [16].

4.1 Interface treatment with the projection operators

If no T–junction interface is present in the mesh, for example in Figure 1a and 1b, the operators \(I_{L2R}^p\) and \(I_{R2L}^p\) in (14) are used to impose grid interface conditions in the same way as the interpolation operators discussed in §3. \(I_{L2R}^p\) and \(I_{R2L}^p\) satisfy an analogue of relation (1) up to tenth order accuracy, and relation (2) up to fourth order accuracy. The stability analysis and accuracy properties of the interpolation operators in §3 are still valid for \(I_{L2R}^p\) and \(I_{R2L}^p\).

If a T–junction interface is present in the mesh, for example in Figure 2, we cannot use \(I_{L2R}^p\) and \(I_{R2L}^p\) in a direct way. Instability occurs around the junction point if on one side the SBP norm has the interior weights while on the other side it has the boundary weights, and no energy estimate can be obtained. To overcome the instability, the coupling is done on the glue grid. That is, we project finite difference solutions to the glue grid, compute the penalty terms there, and project them back to the finite difference grids. In this way, we avoid the instability caused by the SBP norms since the penalty terms are computed on the common glue grid.

The projection technique is very flexible to handle grid interfaces in the sense that we are free to choose the interface structure, the mesh refinement ratio and the accuracy of the diagonal norm SBP operators. In [10], the authors also couple the SBP finite difference method with the discontinuous Galerkin method, inspired by the relation between the discontinuous Galerkin spectral element method and the SBP–SAT finite difference method [5].

Finally, we remark that even with the mesh in Figure 1a where both interpolation technique and projection technique are applicable, the interpolation operators \(I_{2F}(I_{2F})\) are not the same as \(I_{L2R}^p(I_{R2L}^p)\) in (14). The latter one has a wider stencil. In the construction procedure of these operators, one gets a system of linear equations after imposing stability and accuracy requirements. The solution of the linear system has a few free parameters. There are different ways to tune those free parameters. In [16], the free parameters are used to minimize the coefficients of the leading interpolation error in \(L^2\) norm, while in [10] the free parameters are used to minimize the distance between nearest eigenvalues of \(P_{p}\) for a finite difference grid of size 64. The choice of tuning free parameters has no influence on the theoretical order of accuracy, but may have an impact on condition (2) and the practical accuracy. This is studied in more detail in the numerical experiments in §5.

5 Numerical experiments

In this section, numerical experiments are performed to compare the schemes with the interpolation operators and the projection operators, and verify their stability and accuracy properties. Moreover, we also conduct two numerical
experiments to study the efficiency of local mesh refinement by solving the wave equation on a domain with a complex geometry.

The $L_2$ error and maximum error are computed as the norm of the difference between the exact solution $u^{ex}$ and the numerical solution $u^h$ according to

$$\| u^h - u^{ex} \|_{L_2} = \sqrt{h^d (u^h - u^{ex})^T (u^h - u^{ex})},$$

$$\| u^h - u^{ex} \|_{\infty} = \max |u^h - u^{ex}| / \text{amp},$$

where $d$ is the dimension of the equation and amp is the maximum amplitude of the solution. The convergence rate is computed by

$$q = \log \left( \frac{\| u^h - u^{ex} \|}{\| u^{2h} - u^{ex} \|} \right) / \log \left( \frac{1}{2} \right).$$

5.1 Stability study

We begin with an eigenvalue analysis for condition (2). The computational domain is $x \in [-1, 1]$ and $y \in [0, 1]$ with a grid interface at $x = 0$. In the left domain the number of grid points is 26 in both $x$ and $y$ directions, while in the right domain the number of grid points is 51 in both $x$ and $y$ directions. The mesh refinement ratio is $1 : 2$ across the grid interface, which enables both the interpolation operators and projection operators applicable. The matrices $\Xi_L$ and $\Xi_R$ are symmetric, so they have real eigenvalues. We denote $k_L$ and $k_R$ the smallest eigenvalue of $\Xi_L$ and $\Xi_R$ in (2), scaled by the mesh size:

$$k_L = \min(\text{eig}(\Xi_L)) / h_{yL}, \quad k_R = \min(\text{eig}(\Xi_R)) / h_{yR}.$$ 

The reason for the scaling is that the elements in $\Xi_L / \Xi_R$ are proportional to $h_{yL} / h_{yR}$.

In Table 3, we list $k_L$ and $k_R$ for the interpolation operators and the projection operators in Column three and four, respectively. For the interpolation operators, (2) holds for both the second and fourth order accurate cases with errors up to machine precision. For the second order accurate case, we can prove that $k_L, k_R \geq 0$ independent of $h$, because $\Xi_L$ is diagonally dominant and $\Xi_R$ can be transformed to a diagonally dominant matrix without changing the signs of the eigenvalues. For the sixth and eighth order cases, (2) no longer holds. The difference between these two cases is that $k_L$ and $k_R$ are close to zero for the sixth order case, but far away from zero with the eighth order case. When increasing the number of grid points, the values of $k_L$ and $k_R$ remain unchanged.

For the projection operators, (2) also holds also for the second and fourth order accurate cases. For the sixth, eighth and tenth order cases, (2) does not hold anymore but the values of $k_L$ and $k_R$ are close to zero, and they become slightly closer to zero as the mesh is refined.

Another way of analyzing stability through numerical experiments is to write the semidiscretized equation (4) as a system of ordinary differential equations

$$z_{tt} = Qz + F.$$ (15)
### Table 3: 

<table>
<thead>
<tr>
<th>$2p$</th>
<th>IO</th>
<th>PO</th>
<th>IO</th>
<th>PO</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$k_L$</td>
<td>$-6.2 \cdot 10^{-17}$</td>
<td>$-7.7 \cdot 10^{-16}$</td>
<td>$-5.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$k_R$</td>
<td>$-1.0 \cdot 10^{-16}$</td>
<td>$-8.5 \cdot 10^{-16}$</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$k_L$</td>
<td>$-6.7 \cdot 10^{-17}$</td>
<td>$-8.3 \cdot 10^{-16}$</td>
<td>$-5.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$k_R$</td>
<td>$-1.4 \cdot 10^{-16}$</td>
<td>$-6.3 \cdot 10^{-16}$</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$k_L$</td>
<td>$-6.9 \cdot 10^{-1}$</td>
<td>$-7.5 \cdot 10^{-5}$</td>
<td>$-5.0 \cdot 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>$k_R$</td>
<td>$-8.0 \cdot 10^{-1}$</td>
<td>$-8.6 \cdot 10^{-9}$</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>$k_L$</td>
<td>$-3.1 \cdot 10^{1}$</td>
<td>$-4.4 \cdot 10^{4}$</td>
<td>$8.7 \cdot 10^{3}$</td>
</tr>
<tr>
<td></td>
<td>$k_R$</td>
<td>$-7.4 \cdot 10^{4}$</td>
<td>$-4.8 \cdot 10^{4}$</td>
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<tr>
<td>10</td>
<td>$k_L$</td>
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<tr>
<td></td>
<td>$k_R$</td>
<td></td>
<td>$-1.1 \cdot 10^{-3}$</td>
<td></td>
</tr>
</tbody>
</table>

Table 3: IO: interpolation operators, PO: projection operators. Column 3 and 4 correspond to the numerical study of relation (2), and Column 5 and 6 correspond to the eigenvalue analysis of (15).

It is stable if the eigenvalues of $Q$ are real and non–positive. Otherwise, the numerical scheme is unstable. We have computed the eigenvalues of $Q$ by using the same mesh as for the computation of $k_L$ and $k_R$. All the eigenvalues are real. In Table 3, the largest eigenvalue of $Q$ is shown in Column five and six for the schemes with the interpolation operators and projection operators, respectively. For the numerical scheme with the interpolation operators, it is stable for the second, fourth and sixth order cases, and unstable for the eighth order case. For the numerical scheme with the projection operators, it is stable for up to tenth order cases even though relation (2) only holds for up to fourth order scheme. The eigenvalue analysis indicates that (2) is sufficient but not necessary for stability.

### 5.2 Accuracy study

In this section, the convergence of the SBP–SAT method applied to the wave equation (3) with a non–conforming grid interface is investigated. The analytical solution to (3) is manufactured, which means that a closed form is chosen and is used to obtain the initial and boundary data. At the outer boundaries, Dirichlet boundary condition is imposed weakly by the SAT method as described in [18].

#### 5.2.1 A non–conforming grid interface

In the first numerical experiment, the computational domain is $[-1, 1] \times [0, 1]$ where a grid interface is located at $x = 0, y \in [0, 1]$. In the grid refinement level $r = 0$, the numbers of grid points in the left block and right block are $26 \times 26$ and $51 \times 51$. The mesh sizes are halved in both $x$ and $y$ directions when $r$ is increased by one. In this setting, the grid refinement ratio is $1 : 2$, and both the interpolation operators and the projection operators are applicable for the numerical treatment of interface conditions. The fourth order Runge–Kutta
method is used as the time integrator with the step size in time chosen so small that the temporal error is negligible compared with the spatial error.

The manufactured solution to (3) is chosen to be

\[ U(x, y, t) = \cos(5x + 1) \cos(5y + 2) \cos(5\sqrt{2}t + 3). \] (16)

The computational results are shown in Table 4, where \(2p\) and \(r\) in the first two columns denote the order of accuracy and the mesh refinement level, respectively. In Column 3, 4 and 5 the errors in \(L_2\) norm, the convergence rates in \(L_2\) norm and maximum norm are shown for the numerical schemes with the interpolation operators, whereas in Column 6, 7 and 8 the corresponding results obtained by the schemes with the projection operators are shown.

For the scheme with the interpolation operators and time step \(\Delta t = 0.1h\), the convergence rates in \(L_2\) norm are 1, 3 and 4 for the second, fourth and sixth order schemes, respectively. This agrees with our accuracy discussion in §3. Though stability cannot be proved by the energy method for the sixth order accurate case, it seems that for this particular setting the scheme is stable and exhibits the expected convergence rate. Instability occurs when using the eighth order accurate scheme.

With the projection operators, the convergence rate in \(L_2\) norm is one for the second order accurate scheme, and \(p + 1\) for the fourth, sixth, eighth and tenth order accurate schemes, which agrees with the accuracy discussion in §4. We note that though an energy estimate does not exist for the sixth, eighth and tenth order accurate cases, the schemes are stable and converge as expected.

The time step is \(\Delta t = 0.1h\) for \(2p = 2, 4, 6\). With this time step, the tenth order accurate scheme yields slightly lower convergence rate than expected, and the result shown in Table 4 is obtained with \(\Delta t = 0.05h\). The eighth order accurate scheme is a special one, since with \(\Delta t = 0.05h\) it is even unstable. To obtain the results in Table 4, \(\Delta t = 0.025h\) is used as the time step, which indicates that the eighth order accurate semidiscretized equation is stiff. Moreover, the error obtained with the eighth order accurate scheme is larger than the error obtained with the sixth order accurate scheme, except for the finest mesh refinement level.

From Table 4, it is also observed that the errors are similar to each other for the schemes of the same order of accuracy with interpolation operators and projection operators.

### 5.2.2 A T–junction interface

Next, we consider the computational domain \([-1, 1]^2\) that is divided into three mesh blocks as shown in Figure 2a. The interfaces are located at \(x = 0, y \in [-1, 1]\) and \(y = 0, x \in [0, 1]\). In the grid refinement level \(r = 0\), the numbers of grid points in Block 1 (left), Block 2 (right–up) and Block 3 (right–down) are \(28 \times 51, 27 \times 25\) and \(51 \times 50\), respectively. The mesh sizes are halved in both \(x\) and \(y\) directions when \(r\) is increased by one. This partitioning and meshing result in a highly non–conforming grid interface with a close-up shown in Figure 2c. The interface conditions are imposed weakly by the SAT method with the projection operators. To test convergence, (16) is used as the analytical solution.

The computational results are shown in table 5.
<table>
<thead>
<tr>
<th>2p</th>
<th>r</th>
<th>L₂ error</th>
<th>qₐ₂</th>
<th>qₐ₃</th>
<th>L₂ error</th>
<th>qₐ₂</th>
<th>qₐ₃</th>
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</thead>
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<td>2.02·10⁻²</td>
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</tr>
<tr>
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</tr>
<tr>
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Table 4: Convergence of the SBP–SAT scheme for the wave equation with a grid interface. The interface conditions are handled by the interpolation operators (Column 3,4,5) and the projection operators (Column 6,7,8).
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<th>$L_2$ error</th>
<th>$q_{L_2}$</th>
<th>Maximum error</th>
<th>$q_M$</th>
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<td>5.86</td>
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</table>

Table 5: Convergence for the wave equation with a T–junction interface handled by the projection operators.
Figure 3: An example of an acoustic time–harmonic plane wave impinging on a circular inclusion, where the wavelength is much smaller inside the circular inclusion than that outside.

Clearly, \((p + 1)^{th}\) convergence rate in \(L_2\) norm is obtained for \(p = 2, 3, 4, 5\) and first order convergence rate is obtained for \(p = 1\). Here, we observe again that the schemes higher than fourth order accuracy are stable though no energy estimate can be obtained.

5.3 Efficiency study

In many applications, the frequencies of the present waves are given by initial and boundary data, and internal forcing functions. The wavelength of a wave is determined by the ratio between the wave speed of the material in which the wave is traveling and the frequency of the wave. The accuracy of a numerical solution can be stated in terms of how many grid points per wavelength are used to resolve the present waves [11]. A reduction in wave speed confined to a subset of the physical domain yields waves of a shorter wavelength localized in that subset. For accuracy it is therefore necessary to refine the grid to compensate for the shorter present wavelengths. For computational efficiency it is important that this refinement is done only in the subset that constitutes the slower media, since it is only in the slower media that wavelengths are reduced. As an example Figure 3 shows the scattering and diffraction of an acoustic time–harmonic plane wave impinging on a circular region of a slower material, the wavelength is seen to be reduced inside the circular region.

Geometrical features of the physical domain such as a complex boundary or an internal cavity introduce a local radius of curvature. A small local radius of curvature compared with the present wavelengths can imply difficulties when generating a computational grid. As an example Figure 4a shows the scattering of an acoustic time-harmonic plane wave impinging on a circular cavity of a radius of curvature smaller than the wave length of the incoming and scattered waves. A part of the grid used to represent the wave field is shown as an inset, where it is seen in Figure 4b that the quality of the grid is impaired as the grid spacing gets unnecessarily small close to the cavity.

In the preceding experiments it has been verified that using interpolation and
projection operators to patch together the computational grid in a multi–block fashion yields a stable discretization, the convergence rate, however, was seen to be reduced. In the following experiments we investigate the practical benefit of using interpolation operators and projection operators in a region with a slower wave speed or a geometrical feature of a small radius of curvature albeit the order reduction. In particular, we will consider experiments involving acoustic waves impinging on a circular cavity and a circular inclusion of a differing material.

The numerical method used to solve the acoustic wave equation in the following experiments is based on the SBP-SAT scheme described in [27]. The geometrical features are handled by using a multi-block strategy to decompose the physical domain into blocks, where each block allows for a mapping to curvilinear coordinates. In [27] the blocks that constitute the domain are discretized by using conforming grids and patched together by the SAT method. In this paper we allow for non–conforming grids by implementing interpolation operators as well as projection operators into the handling of the multi-block interfaces.

The following numerical experiments use two different two dimensional domains:

- \( D_1 \): An acoustic plane with a circular cavity of radius \( a \).
- \( D_2 \): An acoustic plane with a circular inclusion of radius \( a \).

The geometries of the domains are handled by decomposing each domain in a multi–block fashion. The blocks are then patched together to compound the entire domain. A detailed description of how these two grids are constructed is presented in the Appendix.

5.3.1 A circular cavity

In this numerical experiment, we consider a domain of an infinite homogeneous medium with a circular cavity of radius \( a = 1 \). Let a plane harmonic wave
Figure 5: Computational domain of the circular cavity experiment

\[ u_i = e^{i(\omega t - \gamma x)} \] propagate in that domain and impinge on the cavity. A scattered wave \( u_s \) is generated when the incident wave hits the cavity, and the total displacement \( u_i + u_s \) satisfies the wave equation. Homogeneous Neumann boundary condition is imposed at the cavity boundary. A detailed derivation of an analytical solution is found in [6, §7].

We take \( \omega = 2\pi \) and \( c = 2.5 \), which give a wavelength 2.5. The computational domain \( D_1 \) is chosen to be the rectangular \([-25.5, 11.7] \times [-11.7, 11.7]\) and the cavity is centred at the origin. Two ways of partitioning the domain are considered, namely the N–partitioning and the T–partitioning shown in Figure 5a and 5b, respectively. In the N–partitioning approach, we only use conforming grid interfaces and conforming mesh blocks. The cavity is surrounded by four blocks that constitute the square \([-11.7, 11.7]^2\), which is attached by a rectangular domain to the left. The numbers of grid points on each edge are shown in the figure, and are chosen so that approximately 20 grid points per wavelength are used in the discretization. In this setting, the mesh is of bad quality since the mesh size near the cavity is significantly smaller than that near the outer boundaries. To overcome this drawback, we propose the T–partitioning where the cavity is surrounded by a small square block \([-1.3, 1.3]^2\). Here, all the grid interfaces are also conforming but a T–junction interface is present at \( x = -11.7 \) with the intersection points marked by the dots. Again we choose the mesh size so that there are approximately 20 grid points per wavelength, and here it is only over–resolved in the small block \([-1.3, 1.3]^2\). The T–partitioning results in a mesh of 54903 grid points. The number of grid points with the N–partitioning is about doubled to 109867.

We employ the fourth and sixth order SBP–SAT method to propagate the wave for ten periods, and show the recorded maximum errors in Figure 6a and 6b. In both cases, the maximum error with the T–partitioning is about three times larger than that with the N–partitioning. The is not surprising because the mesh with the T–partitioning has less grid points than the mesh with the N–partitioning, and the corresponding scheme with the T–partitioning has one order lower convergence rate than that of the N–partitioning. It does not seem
to improve the efficiency by using T–junction interfaces for this case.

Although using T–junction interfaces introduces a larger error in the solution, it could be beneficial for a problem with a more complex geometry. For example, if there are several cavities in the domain, an N–partitioning that only allows conforming mesh blocks would produce a large number of small mesh blocks. With a higher order accurate scheme, the boundary stencil gets wider and the number of grid points in each direction must be large enough in every mesh block. It is therefore over–resolved in those small mesh blocks and results in a suboptimal performance of the numerical scheme, and T–junction interfaces could be desirable.

5.3.2 A circular inclusion

Consider a circular domain of radius $a = 1$ embedded in an infinite surrounding medium of differing material with wave speed $c$. Let the wave speed $c'$ of the circular domain be such that $c' < c$ and let an incoming time–harmonic plane wave $u_I(x, y, t) = e^{i(\omega t - \gamma x)}, \gamma = \frac{\omega}{c}$ travel in the $x$–direction and impinge on the circular inclusion. The resulting field consists of the incoming wave $u_I$, as well as the scattered and diffracted waves $u_S$ and $u_D$, respectively. The conditions at the interface of the circular inclusion are

$$u_I + u_S = u_D,$$
$$c \frac{\partial}{\partial n} (u_I + u_S) = c' \frac{\partial}{\partial n} u_D,$$

on $x^2 + y^2 = 1$,  

(17)

where $\frac{\partial}{\partial n}$ denotes the normal derivative on the interface. Since $c' < c$, the short wavelength occurs inside the circular domain. An analytical expression for the solution is given in [1, pp. 667].

In the numerical experiments we take $\omega = 2\pi, c = 1$ and $c' = 1/10$, which give a wavelength of 1 and 1/10 outside and inside the circular inclusion, respectively. To resolve the geometric features, the computational domain is decomposed into 10 conforming blocks as shown in Figure 7. We take the side
length $2D = 2.6$ for the square block outside the circular inclusion, and the side length $2d = 0.7\sqrt{2}$ for the square block inside the circular inclusion. Both square blocks are centered at the origin. The Cartesian block $[-5.9, -1.3] \times [-1.3, 1.3]$ is then attached to the left of this representation. Firstly, we only use conforming grid interfaces with the numbers of grid points in each block given in Table 6. The resolution outside the circular inclusion is about 16 and 51 points per wavelength in the horizontal and vertical direction, respectively. Inside the circular inclusion the waves are resolved by about 10 grid points per wavelength in both directions. Hence, the waves are significantly over–resolved in the vertical direction outside the inclusion, which leads to a suboptimal efficiency of the numerical scheme.

To amend the over–resolution, we partition the computational domain in the same way as above but use non–conforming interfaces denoted by the small red circles in Figure 7. The non–conforming grid interfaces are handled by the interpolation and projection operators. The numbers of grid points in each block are chosen as in Table 7. Now the resolution is reduced to about 26 grid points per wavelength in the vertical direction outside the circular inclusion. The interface conditions (17) are imposed numerically with the SAT technique and at outer boundaries the exact solution is injected at all times. In [4], the SBP finite difference method applied to the wave equation with the injection method to impose the Dirichlet boundary condition is proved to be stable.

The solution is propagated numerically for 10 temporal periods by the SBP–SAT method and the relative maximum error is recorded at each time step. In Figures 8a and 8b we plot the recorded relative maximum error as functions of time. Here we see that the errors are similar in both cases. The grid with conforming interfaces has 46460 grid points, whereas the grid with non–conforming interfaces has 38710 grid points. The smallest grid size is determined by the resolution inside the circular inclusion, for this reason the time step $\Delta t = 4 \times 10^{-4}$ for the sixth order SBP-SAT method and $\Delta t = 5 \times 10^{-4}$ for the fourth order SBP-SAT method are the same for both grids. We conclude that even though the formal order of accuracy is lowered by using blocks with non-conforming
interfaces it can be a beneficial strategy within the SBP-SAT framework when
the physical domain contains regions that require a higher density of grid points.
We also note that for more complex multi–block domains consisting of a larger
number of blocks the benefits of using blocks with non–conforming grid inter-
faces are expected to increase.

In the experiment with the sixth order SBP–SAT scheme with the interpola-
tion operators, the numerical solution blows up quickly, which indicates that the
scheme is unstable. The corresponding scheme with the projection operators is
stable. According to the stability analysis in §5.1, for the sixth order accurate
scheme condition (2) holds for neither the interpolation operator nor the pro-
jection operator. If the smallest eigenvalue of $\Xi_{L/R}$ is non–negative, then an
energy estimate exists that ensures stability. The smallest eigenvalue of $\Xi_{L/R}$
scaled by the mesh size is in the magnitude of $10^{-1}$ for the sixth order accu-
rate interpolation operators, and $10^{-5}$ for the sixth order accurate projection
operators. The violation of (2) is much weaker for the projection operator than
for the interpolation operator, which explains the observation in the numerical
experiments.

Table 6: Number of grid points with conforming grid interfaces

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<th>$N_\eta$</th>
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<td>101</td>
</tr>
<tr>
<td>$B_1^{(1)} - B_4^{(1)}$</td>
<td>101</td>
<td>26</td>
</tr>
<tr>
<td>$B_1^{(2)} - B_3^{(2)}$</td>
<td>101</td>
<td>51</td>
</tr>
<tr>
<td>$B_5^{(2)}$</td>
<td>101</td>
<td>101</td>
</tr>
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</table>

Table 7: Number of grid points with non–conforming grid interfaces

<table>
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<th>Block</th>
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<th>$N_\eta$</th>
</tr>
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<td>$B_0$</td>
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<tr>
<td>$B_1^{(1)} - B_4^{(1)}$</td>
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<td>26</td>
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<td>$B_1^{(2)} - B_3^{(2)}$</td>
<td>101</td>
<td>51</td>
</tr>
<tr>
<td>$B_5^{(2)}$</td>
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</tr>
</tbody>
</table>

Figure 8: Maximum error of the numerical experiment with the circular inclu-
sion
6 Conclusion and outlook

In this work, high order accurate SBP finite difference operators are used to discretize the wave equation in the second order form on a block-structured mesh. Adjacent mesh blocks are patched together by imposing suitable interface conditions via the SAT technique. The emphasis is placed on the numerical treatment of non-conforming grid interfaces by the interpolation operators and projection operators, which are also compared in terms of the stability and accuracy properties. In contrast to first order hyperbolic equation, stability of the scheme for the second order wave equation introduces an extra condition on the numerical treatment of non-conforming grid interfaces. This condition is satisfied for the second and fourth order accurate cases, and an energy estimate is derived to ensure stability. For higher order accurate schemes, the extra stability condition is violated. We show by the eigenvalue analysis that the violation is stronger with interpolation operators than with projection operators. Unphysical growths are observed in the numerical experiments with high order interpolation operators, whereas with projection operators the scheme is stable in all the experiments we have conducted.

We have also performed a truncation error analysis and an investigation of the convergence property for the scheme, which indicates that the convergence rate is one order lower than that in the corresponding case with conforming grid interfaces. This is verified in numerical experiments. The efficiency studies show that for a problem with a very complex geometry, it could be beneficial to use non-conforming grid interfaces.

For high order accurate interpolation operators and projection operators, there are free parameters left in the construction process. It is desirable to tune the free parameters so that the extra stability condition is satisfied. However, the resulting nonlinear problem seems difficult to solve. To overcome the accuracy reduction, more accurate interpolation operators or new ways of imposing interface conditions are needed.

Appendix

We give a detailed description for the construction of the two grids used in the efficiency studies in §5.3. A general block $B_i$ of a decomposition has four boundaries defined by the parametrized curves

\[
C_{iS} = (x_{iS}(\xi), y_{iS}(\xi)), \quad C_{iN} = (x_{iN}(\xi), y_{iN}(\xi)), \\
C_{iW} = (x_{iW}(\eta), y_{iW}(\eta)), \quad C_{iE} = (x_{iE}(\eta), y_{iE}(\eta)),
\]

where $0 \leq \xi \leq 1, 0 \leq \eta \leq 1$. $C_{iS}$ and $C_{iN}$ describe one pair of opposing sides and $C_{iW}$ and $C_{iE}$ the other pair. Let $P_{iSW}$ denote the point of intersection between the curves $C_{iS}$ and $C_{iW}$ e.t.c. A bijection $(x, y) = \mathcal{T}_i(\xi, \eta)$ from the unit square $S = [0,1]^2$ to the block $B_i$ of the decomposition is given by the transfinite interpolation [9] as

\[
\mathcal{T}_i(\xi, \eta) = (1 - \eta)C_{iS} + \eta C_{iN} + (1 - \xi)C_{iW} + \xi C_{iE} \\
- \xi \eta P_{iNE} - \xi(1 - \eta)P_{iSE} - \eta(1 - \xi)P_{iNW} - (1 - \xi)(1 - \eta)P_{iSW}.
\]
The unit square $S$ is discretized by the points

$$\xi_j = jh_\xi, h_\xi = 1/(N_\xi - 1), j = 0, \ldots, N_\xi - 1,$$

$$\eta_k = kh_\eta, h_\eta = 1/(N_\eta - 1), k = 0, \ldots, N_\eta - 1,$$

where $N_\xi$ and $N_\eta$ are integers determining the number of grid points in the spatial directions of the discretization of the block $B_i$. The corresponding grid points are computed as

$$(x_j, y_k) = T_i(\xi_j, \eta_k).$$

We now give details on how the grids in $D_1 - D_2$ are constructed. $D_1$ represents a circular cavity in an infinite surrounding media. We construct the computational grid such that the cavity of radius $a$ is centered inside a square of side $2D$. This is done by introducing four blocks $B_1^{(1)} - B_4^{(1)}$. The bounding curves of block $B_1^{(1)}$ are given by

$$C_{1S}^{(1)} = a \left( \xi \sqrt{2} - 1/\sqrt{2}, \sqrt{1 - (\xi \sqrt{2} - 1/\sqrt{2})^2} \right),$$

$$C_{1N}^{(1)} = (D, 2D \xi - D),$$

$$C_{1W}^{(1)} = \left( -\eta(D - a/\sqrt{2}) - a/\sqrt{2}, \eta(D - a/\sqrt{2}) + a/\sqrt{2} \right),$$

$$C_{1E}^{(1)} = \left( \eta(D - a/\sqrt{2}) + a/\sqrt{2}, \eta(D - a/\sqrt{2}) + a/\sqrt{2} \right).$$

The bounding curves of the remaining blocks $B_2^{(1)} - B_4^{(1)}$ that constitute the square with the cavity at the center are obtained via rotation by a factor $\pi/2$,

$$C_{ij}^{(1)} = C_{i-1j}^{(1)} \begin{bmatrix} \cos \pi/2 & -\sin \pi/2 \\ \sin \pi/2 & \cos \pi/2 \end{bmatrix}, \quad i = 2, 3, 4, \quad j = S, N, W, E. \quad (18)$$

The domain $D_1$ can now be represented by attaching the grid representing the cavity to one or more Cartesian blocks.

The circular inclusion of $D_2$ is decomposed into five blocks $B_1^{(2)} - B_5^{(2)}$. The block $B_1^{(2)}$ is a square at the center of the circular inclusion with corners at the points $(\pm ad, \pm ad), 0 < d < \sqrt{2}/2$ defined by the bounding curves,

$$C_{1S}^{(2)} = a \left( 2d\xi - d, -d \right), \quad C_{1N}^{(2)} = a \left( 2d\xi - d, d \right),$$

$$C_{1W}^{(2)} = a \left( -d, 2d\eta - d \right), \quad C_{1E}^{(2)} = a \left( d, 2d\eta - d \right).$$

Here $a$ is the radius of the circular inclusion. The block $B_2^{(2)}$ is defined by its bounding curves,

$$C_{2S}^{(2)} = C_{1N}^{(2)},$$

$$C_{2N}^{(2)} = C_{1S}^{(2)},$$

$$C_{2W}^{(2)} = a \left( -\eta(\sqrt{2}/2 - d) - d, \eta(\sqrt{2}/2 - d) + d \right),$$

$$C_{2E}^{(2)} = a \left( \eta(\sqrt{2}/2 - d) + d, \eta(\sqrt{2}/2 - d) + d \right).$$
The bounding curves of the remaining blocks $B_3^{(2)}$–$B_5^{(2)}$ that constitute the circular inclusion of $D_2$ are obtained via rotations by a factor $\pi/2$ as in (18). The inclusion is then centered inside a square of side $2D$ by attaching it to the blocks $B_1^{(1)}$–$B_4^{(1)}$ above. The circular inclusion is now the union of the nine blocks $B_1^{(1)}$–$B_4^{(1)}$ and $B_1^{(2)}$–$B_5^{(2)}$. The domain $D_2$ can now be represented by attaching the grid representing the inclusion to one or more Cartesian blocks.

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