Energy Stable and High-order-accurate Finite Difference Methods on Staggered Grids

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Abstract

For wave propagation over distances of many wavelengths, high-order finite difference methods on staggered grids are widely used due to their excellent dispersion properties. However, the enforcement of boundary conditions in a stable manner and treatment of interface problems with discontinuous coefficients usually pose many challenges. In this work, we construct a provably stable and high-order-accurate finite difference method on staggered grids that can be applied to a broad class of boundary and interface problems. The staggered grid difference operators are in summation-by-parts form and when combined with a weak enforcement of the boundary conditions, lead to an energy stable method on multiblock grids. The general applicability of the method is demonstrated by simulating an explosive acoustic source, generating waves reflecting against a free surface and material discontinuity.

1. Introduction

Some of the most popular numerical methods for wave propagation problems are high-order finite difference methods on staggered grids. These methods include Yee’s method for solving Maxwell’s equations \cite{Yee} and the velocity-stress formulation for solving the elastic wave equation \cite{Aki, Kanamori, Mavko, Nur}. Although

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a few decades have past since the introduction of these methods, they are still actively and widely used today. This widespread success is because of the simplicity, accuracy, and computational efficiency of these methods.

High-order methods have excellent dispersion properties which enables accurate wave propagation over long distances using relatively few grid points per wavelength compared to low-order methods. Another aspect that influences the dispersion properties of a scheme is the arrangement of unknowns in the grids. In staggered grid methods, the unknowns are arranged on different grids, whereas in collocated grid methods, the unknowns are arranged together at the nodes of a single grid. The use of staggered grids results in superior dispersion properties compared to collocated grids. Figure 1 shows the dispersion curves of collocated and staggered central, schemes for a few different orders of accuracy, demonstrating the advantage of staggered grids.

![Dispersion Curves](image)

Figure 1: Dispersion curves for the collocated and staggered finite difference approximations of the wave equation $\frac{\partial p}{\partial t} + u_x = 0$, $u_t + p_x = 0$ for $x \in [0, 1]$ subject to periodic boundary conditions. Dispersion curves are obtained by inserting the modal representation $u_j(t) = u(x_j, t) = \exp(ikx_j - \omega t)$, into the semi-discrete approximation. Here, $k = 2\pi m$ ($m = 0, \pm 1, \ldots, N/2) \text{ assuming } N \text{ even, and } x_j = jh$, for $j = 0, 1, \ldots, N$ where $h = 1/N$ is the grid spacing. The legend states the order of accuracy (second, fourth, \ldots) of each approximation. The black line is the exact dispersion relation.

The main drawbacks of the staggered grid finite difference method are the difficulty of implementing stable boundary conditions and treating complex geometry - in particular for high-order accuracy. Unless the semi-discrete
approximation satisfies an energy estimate, non-physical energy growth in
time can occur and destroy the accuracy of the solution. One way to prevent
non-physical energy growth in time is to use Summation-By-Parts (SBP)
difference operators [6, 7, 8, 9] and weakly enforce the boundary conditions
via the Simultaneous-Approximation-Term (SAT) technique [10]. SBP op-
erators satisfy a summation-by-parts property that mimics integration by
parts. This property is essential for obtaining an energy estimate, but is in
its standard form restricted to collocated grids. In this work we extend the
SBP-SAT approach to staggered grids by introducing a new summation-by-
parts property.

There are many advantages of extending the SBP-SAT approach to stag-
nered grids. With this development in hand, one can construct stable, dual
consistent difference approximations which is important for adjoint problems
[11, 12]. One can also gain geometric flexibility by coupling structured grids
to unstructured grids in a provably stable manner, e.g., using finite volume
methods [13, 14, 15], or discontinuous Galerkin methods [16]. To take ad-
vantage of many of these benefits, one only has to modify the boundary
procedures in existing staggered grid codes.

This paper is organized as follows. Section 2 defines SBP operators on
staggered grids. Section 3 and Section 4 use these definitions to solve the wave
equation in one and two dimensions subject to linear boundary conditions.
Section 5 is dedicated to performing a series of numerical experiments to
assess the accuracy of the new SBP staggered grid operators and showcase
some of their capabilities. In particular, we consider singular source terms to
set off explosions, and solve problems with material discontinuities. Finally,
in Section 6 conclusions are drawn.

2. Definitions

In this section, we construct SBP high-order finite difference operators
on staggered grids. We discretize the interval \( x \in [0, 1] \) using the grid points

\[
x_j = jh, \quad 0 \leq j \leq N, \quad \text{and} \quad x_{j-1/2} = (j - 1/2)h, \quad 1 \leq j \leq N,
\]

where \( h = 1/N \) is the grid spacing. Let the staggered grids be defined as

\[
x_+ = [x_0, \ x_1, \ldots, \ x_N]^T \in \mathbb{R}^{N+1}
x_- = [x_0, \ x_{1/2}, \ldots, \ x_{N-1/2}, \ x_N]^T \in \mathbb{R}^{N+2}.
\]
Figure 2: Illustration of second-order accurate difference approximations on staggered grids.

Thus, both grids contain the endpoints $x_0 = 0$ and $x_N = 1$.

SBP staggered grid finite difference operators are constructed by using central difference approximations at interior points and one-sided difference approximations at boundary points. For example, second-order accuracy in the interior is given by the standard central difference approximations

$$
\left. \frac{d\psi}{dx} \right|_{x_i} \approx \frac{\psi_{i+1/2} - \psi_{i-1/2}}{h}, \quad \left. \frac{d\phi}{dx} \right|_{x_{i+1/2}} \approx \frac{\phi_i - \phi_{i+1}}{h},
$$

for smooth grid functions $\psi$ and $\phi$ defined on $x_-$ and $x_+$, respectively.

We store the difference approximations in matrices $D_+ \in \mathbb{R}^{(N+1)\times(N+2)}$, $D_- \in \mathbb{R}^{(N+2)\times(N+1)}$. The difference operator $D_+$ acts on a grid function defined on $x_-$, but approximates its derivative on $x_+$. Similarly, the difference operator $D_-$ acts on a grid function defined on $x_+$, but approximates its derivative on $x_-$. Figure 2 demonstrates the way in which the difference operators act on the grid functions for second-order accuracy. SBP staggered grid operators are defined as follows.

**Definition 1.** The difference operators $D_+ = P_+^{-1}Q_+$ and $D_- = P_-^{-1}Q_-$ are SBP staggered grid difference operators if the following properties hold:

1. $P_+$ and $P_-$ are diagonal and positive definite matrices defining the respective discrete $L_2$ norms

$$
\|\phi\|_h^2 = \phi^T P_+ \phi \approx \int_{x_0}^{x_{1/2}} \phi^2 dx, \quad \|\psi\|_h^2 = \psi^T P_- \psi \approx \int_{x_{N-1/2}}^{x_N} \psi^2 dx,
$$

for smooth grid functions $\phi$ defined on $x_+$ and $\psi$ defined on $x_-$.
(ii) The matrices $Q_+$ and $Q_-$ satisfy the SBP property

$$Q_+ + Q_-^T = B_+ = B_-^T = B,$$

where the matrix $B$ restricts the grid functions to the boundary: $\phi^T B \psi = \phi_N \psi_N - \phi_0 \psi_0$.

The properties (i) and (ii) in Definition 1 are satisfied by construction. The order of accuracy of the SBP staggered grid operators is $s$ for boundary points and $2s$ for interior points. We have the accuracy relations

$$D_+ \psi = R_+ \quad \text{and} \quad D_- \phi = R_-,$$

for smooth functions $\psi$ and $\phi$. The residuals satisfy

$$R_+ = h[\mathcal{O}(h^s), \ldots, \mathcal{O}(h^s), \mathcal{O}(h^{2s}), \ldots, \mathcal{O}(h^s)]^T,$$
$$R_- = h[\mathcal{O}(h^s), \ldots, \mathcal{O}(h^s), \mathcal{O}(h^{2s}), \ldots, \mathcal{O}(h^s), \ldots, \mathcal{O}(h^s)]^T.$$

When we refer to the order of accuracy of the SBP operators, we shall refer to the interior order of accuracy. For example, a pair of second-order accurate SBP staggered grid operators is

$$Q_+ = \begin{bmatrix}
-\frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\
-\frac{1}{2} & -\frac{1}{4} & \frac{3}{4} \\
& & & \\
& & & -1 & 1 \\
& & & & & \ddots & \ddots \\
& & & & & & -1 & 1 \\
& & & & & & -\frac{3}{4} & \frac{1}{2} & \frac{1}{2} \\
& & & & & & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} \\
\end{bmatrix},$$

$$Q_- = \begin{bmatrix}
-\frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\
-\frac{1}{2} & -\frac{1}{4} & \frac{3}{4} \\
& & & \\
& & & -1 & 1 \\
& & & & & \ddots & \ddots \\
& & & & & & -1 & 1 \\
& & & & & & -\frac{3}{4} & \frac{1}{2} & \frac{1}{2} \\
& & & & & & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} \\
\end{bmatrix}.$$
and

\[ P_+ = \text{diag} \left( \left[ \frac{1}{2}, 1, \ldots, 1, \frac{1}{2} \right] \right) h, \]

\[ P_- = \text{diag} \left( \left[ \frac{1}{2}, \frac{1}{4}, \frac{5}{4}, 1, \ldots, 1, \frac{5}{4}, \frac{1}{4}, \frac{1}{2} \right] \right) h. \]

However, the accuracy at the boundary points is first-order.

3. Analysis in one dimension

In this section, we use the SBP staggered grid operators to construct a stable, semi-discrete approximation of the wave equation. Stability is shown by deriving a discrete energy estimate and weakly enforcing the boundary conditions.

3.1. Continuous problem

As a model problem, consider the wave equation in one dimension:

\[ \frac{\partial p}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad \frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} = 0, \quad 0 \leq x \leq 1, \quad t \geq 0. \quad (4) \]

We apply the energy method \[17\], which leads to

\[ \frac{1}{2} \frac{d}{dt} (\| p \|^2 + \| u \|^2) = -pu \big|_{x=0}^1, \quad (5) \]

where \( \| p \|^2 = \int_0^1 p^2 dx \). For simplicity, consider only the boundary at \( x = 0 \). The number and form of boundary conditions are determined by a diagonalization. The right-hand side in \[5\] is written as a quadratic form:

\[ pu \big|_{x=0} = \frac{1}{2} U^T A U \big|_{x=0}, \quad U = \begin{bmatrix} p \\ u \end{bmatrix}, \quad A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad (6) \]

which is diagonalized by

\[ A = X \Lambda X^T, \quad X = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \Lambda = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}. \quad (7) \]

By inserting \[7\] into \[5\], we obtain

\[ \frac{d}{dt} (\| p \|^2 + \| u \|^2) = w^T \Lambda w \big|_{x=0} = (w^+)^2 \big|_{x=0} - (w^-)^2 \big|_{x=0}, \quad (8) \]
where \( w = [w^-, w^+]^T \), \( w^\pm = (X^\pm)^T U \) are the incoming and outgoing characteristic variables, \( \Lambda = \text{diag}([\Lambda^-, \Lambda^+]^T) \) contains the positive and negative eigenvalues, and \( X = [X^-, X^+] \) are the corresponding eigenvectors, respectively. The characteristic variables are

\[
    w^- = \frac{u - p}{\sqrt{2}} \quad \text{and} \quad w^+ = \frac{u + p}{\sqrt{2}}. \tag{9}
\]

The number of boundary conditions needed is equal to the number of positive eigenvalues. Since \( \Lambda^+ \) contains precisely one positive eigenvalue, one boundary condition must be imposed. We consider a linear homogeneous boundary condition of the form

\[
    LU|_0 = w^+|_0 - rw^-|_0 = 0, \tag{10}
\]

for a given reflection coefficient \( r \), where the boundary operator is

\[
    L = \frac{1}{\sqrt{2}} (1 + r, 1 - r)^T. \tag{11}
\]

Finally, by imposing the boundary condition, (8) becomes

\[
    \frac{d}{dt} (\|u\|^2 + \|p\|^2) = w^T \Lambda w|_0 = (w^+)^T \Lambda^+ w^+|_0 + (w^-)^T \Lambda^- w^-|_0 = - (1 - r^2)(w^-)^2|_0, \tag{12}
\]

and we have an estimate for \(|r| \leq 1\).

3.2. The semi-discrete approximation

Next, we use the results from the continuous analysis to construct a stable, semi-discrete approximation of the problem (4).

Consider the semi-discrete approximation

\[
    u_t + D_+ p = \sigma_1 P_+^{-1} e_{0+} (w_0^+ - r w_0^-), \tag{13}
\]

\[
    p_t + D_- u = \sigma_2 P_-^{-1} e_{0-} (w_0^+ - r w_0^-).
\]

In (13), the grid functions \( u \) and \( p \) are stored on the \( x_+ \) and \( x_- \) grids, respectively. The right-hand side contains penalty terms that weakly enforce the boundary condition (10). The penalty terms are restricted to the boundary using: \( u_0 = e_{0+}^T u \) and \( p_0 = e_{0-}^T p \). The parameters \( \sigma_1 \) and \( \sigma_2 \) will be determined for stability. For simplicity, as in the previous section, we have neglected the boundary condition at \( x = 1 \). The characteristic variables \( w^+ \) and \( w^- \) are defined using (9).
Proposition 1. The semi-discrete approximation (13) of (4) with boundary condition (10) is stable if
\[ \sigma_1 = -\frac{1}{\sqrt{2}} \quad \text{and} \quad \sigma_2 = -\frac{1}{\sqrt{2}}, \] (14)

Proof. We apply the discrete energy method to (13). By using the SBP property (3), we get
\[ \frac{1}{2} d\|p\|_h^2 + \frac{1}{2} d\|u\|_h^2 = \frac{1}{2} U_0^T A U_0 + U_0^T \Sigma (w_0^+ - r w_0^-), \] (15)
where \( \|p\|_h^2 = p^T P_- p \) and \( \|u\|_h^2 = u^T P_+ u \), and \( p_0 v_0 \) has been replaced by \( U_0^T A U_0 / 2 \) using (6), and \( \Sigma = [\sigma_1, \sigma_2]^T \). By diagonalizing \( A \) using (7) and performing the substitution \( W = X^T U \), we get
\[ \frac{1}{2} d\|p\|_h^2 + \frac{1}{2} d\|u\|_h^2 = \frac{1}{2} (w_0^+)^2 - \frac{1}{2} (w_0^-)^2 + W_0^T X^T \Sigma (w_0^+ - r w_0^-). \] (16)

The choice \( \Sigma = -X \Lambda^+ = -[1, 1]^T / \sqrt{2} \) yields \( W_0^T X^T \Sigma = -w_0^+ \), and
\[ \frac{d}{dt} (\|p\|_h^2 + \|u\|_h^2) = (w_0^+)^2 - (w_0^-)^2 - 2 w_0^+ (w_0^+ - r w_0^-) \]
\[ = -(w_0^+)^2 - (w_0^-)^2 + 2 r w_0^+ w_0^- + r^2 (w_0^-)^2 - r^2 (w_0^-)^2 \]
\[ = -(1 - r^2)(w_0^-)^2 - (w_0^+ - r w_0^-)^2 \leq 0, \quad |r| \leq 1. \] (17)

The result is similar to (12), but also includes numerical dissipation that vanishes with grid refinement.

4. Analysis in two dimensions

In this section we extend the previous analysis to two dimensions.

4.1. Continuous problem

In two dimensions, the wave equations becomes
\[ \frac{\partial p}{\partial t} + \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad \frac{\partial u}{\partial t} + \frac{\partial p}{\partial x} = 0, \quad \frac{\partial v}{\partial t} + \frac{\partial p}{\partial y} = 0, \quad (x, y) \in \Omega, \ t \geq 0. \] (18)

The energy method applied to (18) leads to
\[ \frac{1}{2} d\|p\|^2 + \frac{1}{2} d\|u\|^2 + \frac{1}{2} d\|v\|^2 = - \int_{\partial \Omega} p u_n ds, \] (19)
where \( u_n = u\hat{n}_1 + v\hat{n}_2 \) is the normal velocity, \( \hat{n} = [\hat{n}_1, \hat{n}_2]^T \) is the outward-pointing unit normal associated with the boundary \( \partial\Omega \), and \( ds \) is the infinitesimal line element. To determine the number and form of boundary conditions, we first define \( U = [p, -u_n]^T \). Then (19) becomes

\[
\frac{d}{dt} (\|p\|^2 + \|u\|^2 + \|v\|^2) = \oint_{\partial\Omega} U^T AU ds,
\]

where \( A \) is given in (6).

The incoming and outgoing characteristic variables are given by

\[
w^+ = -\frac{1}{\sqrt{2}}(p + u_n), \quad w^- = \frac{1}{\sqrt{2}}(p - u_n).
\]

Again, we consider linear and homogeneous boundary conditions of the form

\[
LU|_{\partial\Omega} = w^+|_{\partial\Omega} - rw^-|_{\partial\Omega} = 0
\]

where the boundary operator is

\[
L = \frac{1}{\sqrt{2}} (1 + r, (r - 1)\hat{n}_1, (r - 1)\hat{n}_2)^T.
\]

Once the boundary conditions have been enforced, (20) becomes

\[
\frac{d}{dt} (\|p\|^2 + \|u\|^2 + \|v\|^2) = -\oint_{\partial\Omega} (1 - r^2)(w^-)^2 ds,
\]

which is bounded for \(|r| \leq 1\).

4.2. The semi-discrete approximation

A semi-discrete approximation of (18) enforcing the boundary condition (21) on the south boundary is (the other boundaries are treated in a analogous manner)

\[
\begin{align*}
\frac{dp}{dt} + (D_{x-} \otimes I_{y-})u + (I_{x-} \otimes D_{y-})v &= \sigma_1 (P_{x-} \otimes P_{y-})^{-1} E_{S,p}^T H_x (w^+_S + rw^-_S), \\
\frac{du}{dt} + (D_{x+} \otimes I_{y-})p &= 0, \\
\frac{dv}{dt} + (I_{x-} \otimes D_{y+})p &= \sigma_2 (P_{x-} \otimes P_{y+})^{-1} E_{S,v}^T H_x (w^+_S + rw^-_S).
\end{align*}
\]
In (24), the grid functions $p$, $u$, and $v$ are stored in vectors having $y$ as the contiguous direction and their arrangement is shown in Figure 3. The difference operators are extended to two dimensions by using the Kronecker product $\otimes$. The identity matrices $I_{x+}$ etc. have the same dimension as the number of grid points in the coordinate direction, indicated by the subscript.

Figure 3: Staggered grid arrangement of unknowns for the semi-discrete approximation of the wave equation in (24).

On the south boundary, the normal velocity is $u_n(x,0,t) = -v(x,0,t)$ and the characteristic variables are:

$$w^+_S = -\frac{1}{\sqrt{2}}(p_S - v_S), \quad w^-_S = \frac{1}{\sqrt{2}}(p_S + v_S). \quad (25)$$

We do not weakly enforce the boundary condition in the second equation (involving $u$), because $u$ is not part of the characteristic variables, on the south boundary. The restriction of the solution to the boundary is obtained using

$$p_S = E_{S,p} p, \quad v_S = E_{S,v} v, \quad E_{S,p} = I_{x-} \otimes e^{T}_{y_0-}, \quad E_{S,v} = I_{x-} \otimes e^{T}_{y_0+}. \quad (26)$$

The stability of the semi-discrete approximation is addressed in the following proposition.

**Proposition 2.** The semi-discrete approximation (24) of (18) with boundary condition (21) is stable if

$$\sigma_1 = -\frac{1}{\sqrt{2}} \quad \text{and} \quad \sigma_2 = -\frac{1}{\sqrt{2}}. \quad (27)$$
Proof. As before, the result follows from applying the discrete energy method. By defining the discrete energy

$$E_h = \frac{1}{2} p^T (P_{x-} \otimes P_{y-}) p + \frac{1}{2} u^T (P_{x+} \otimes P_{y-}) u + \frac{1}{2} v^T (P_{x-} \otimes P_{y+}) v \quad (28)$$

and using the semi-discrete approximation (24), we have

$$\frac{dE_h}{dt} = -p^T (Q_{x-} \otimes P_{y-}) u - p^T (P_{x-} \otimes Q_{y-}) v - u^T (Q_{x+} \otimes Q_{y-}) p$$

$$- v^T (P_{x-} \otimes Q_{y+}) p + (\sigma_1 p_S + \sigma_2 v_S)^T P_{x-} (u^+_S + rw^-_S). \quad (29)$$

By using the SBP property (3) and neglecting terms for all boundaries except the south boundary, we get

$$\frac{dE_h}{dt} = p^T S P_{x-} v_S + (\sigma_1 p_S + \sigma_2 v_S)^T P_{x-} (w^+_S + rw^-_S). \quad (30)$$

The choice $\sigma_1 = \sigma_2 = -1/\sqrt{2}$ leads to

$$\frac{dE_h}{dt} = \frac{1}{2} (r^2 - 1) (w^-_S)^T P_{x-} w^-_S - \frac{1}{2} (w^+_S + rw^-_S)^T P_{x-} (w^+_S + rw^-_S) \leq 0, \quad (31)$$

for $|r| \leq 1$. \qed

5. Numerical experiments

In this section, we conduct numerical experiments to assess the order of accuracy and dispersion properties using a manufactured solution. We also propagate waves due to point sources and treat discontinuous material properties using the multiblock capability of the SBP-SAT approach.

We advance in time using a 4th-order Runge-Kutta method and a time step $\Delta t = \text{CFL} \, h$, where $\text{CFL} = 0.5$. To measure the error, we define $\|e\|_h = \|U - U^*\|_h$, where $U$ is the numerical solution and $U^*$ is computed from a manufactured solution, evaluated at the grid points. The convergence rate is defined as

$$q = \log \left( \frac{\|e\|_{h_1}/\|e\|_{h_2}}{\log (h_1/h_2)} \right), \quad (32)$$

where $h_2 = h_1/2$. 

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5.1. Convergence rate

This test demonstrates that both the collocated and staggered grid SBP-SAT schemes converge at the expected theoretical order of accuracy assuming smooth solutions.

Let \( \Omega = [0, 1] \times [0, 1] \) be the computational domain and let

\[
\begin{align*}
p(x, y, t) &= \sin(kx) \sin(ky) \cos(k\sqrt{2}t), \\
u(x, y, t) &= -\frac{1}{\sqrt{2}} \cos(kx) \sin(ky) \sin(k\sqrt{2}t), \\
v(x, y, t) &= -\frac{1}{\sqrt{2}} \sin(kx) \cos(ky) \sin(k\sqrt{2}t),
\end{align*}
\]

be the manufactured solution. In this test, we specify the incoming characteristic variable and use the manufactured solution as boundary data. We use \( N \) number of grid points in each direction and \( k = 2\pi \). Tables 1-2 lists the convergence rate at \( t = 1 \) of the collocated and the staggered scheme, respectively. Both schemes converge at least at the expected rate of \( s + 1 \), where \( 2s \) is the interior accuracy \([18]\). The SBP staggered grid operators are available at github.com/ooreilly/sbp. Theoretical results related to the construction of these operators will be presented in a forthcoming paper.

<table>
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<th>( N )</th>
<th>2\textsuperscript{nd} ( l^2 ) error</th>
<th>q</th>
<th>4\textsuperscript{th} ( l^2 ) error</th>
<th>q</th>
<th>6\textsuperscript{th} ( l^2 ) error</th>
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Table 1: Staggered SBP operators. Errors and convergence rates.

5.2. Dispersion error

In this experiment, we investigate the dispersion properties of the scheme. Dispersion errors are most noticeable once the solution has propagated over many wavelengths. This effect can be seen by using periodic boundary conditions. The manufactured solution \([33]\) with \( k = 2\pi \) is periodic by construction, and therefore used again.
We advance in time until $t = 1000$ to investigate the error growth in time due to dispersion errors. The error is controlled by choosing $kh \leq \pi$ ($kh = \pi$ triggers the Nyquist mode). Figure 4 shows the error growth in time. The staggered scheme outperforms the collocated scheme in each case.

<table>
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<th>$q$</th>
<th>$4^{th}$  $l^2$ error</th>
<th>$q$</th>
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<td>$4.63 \times 10^{-4}$</td>
<td>4.42</td>
</tr>
<tr>
<td>64</td>
<td>$9.23 \times 10^{-3}$</td>
<td>2.00</td>
<td>$2.63 \times 10^{-4}$</td>
<td>3.03</td>
<td>$1.99 \times 10^{-5}$</td>
<td>4.54</td>
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<tr>
<td>128</td>
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<td>1.96</td>
<td>$3.21 \times 10^{-5}$</td>
<td>3.03</td>
<td>$7.78 \times 10^{-7}$</td>
<td>4.67</td>
</tr>
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<td>256</td>
<td>$5.98 \times 10^{-4}$</td>
<td>1.99</td>
<td>$4.02 \times 10^{-6}$</td>
<td>3.00</td>
<td>$4.18 \times 10^{-8}$</td>
<td>4.22</td>
</tr>
</tbody>
</table>

Table 2: Collocated SBP operators. Errors and convergence rates.

5.3. Singular source term

A staggered grid difference method offers the ability to discretize a singular source term without introducing any spurious oscillations. In this section,
we confirm that the SBP staggered grid operators also possess this property.

On the top boundary of the domain $\Omega = [0, 2] \times [0, 1]$, we specify the boundary condition

$$p(x, 1, t) = g(t)\delta(x - x_\ast). \quad (34)$$

Here, $\delta(x - x_\ast)$ is the Dirac delta function, defined as

$$\int_{-\infty}^{\infty} f(x)\delta(x - x_\ast)dx = f(x_\ast), \quad (35)$$

for some smooth function $f(x)$. We discretize $\delta(x - x_\ast)$ by using the SBP quadrature rule [2]. An approximation of (35) becomes

$$f^T H d = \mathcal{L}_T^T f, \quad (36)$$

where $d$ discretizes the source, and the matrix $\mathcal{L}_x$ restricts the grid function $f$ to $x_\ast$. In the simplest case, if $x_\ast$ coincides with a grid point $x_{k+1/2}$ in the interior, then we have

$$d_{j+1/2} = \begin{cases} \frac{1}{h}, & j = k, \\ 0, & j \neq k. \end{cases} \quad (37)$$

Otherwise, $d$ can be constructed using interpolation. For collocated SBP schemes, the source discretization (37) produces spurious oscillations, see [19] for a solution to this problem.

For simplicity, we require that the source term location $x_\ast$ coincides with the grid point in the middle of the boundary ($x_\ast = 1$). As the source time function in (34), we use the Gaussian

$$g(t) = \exp \left( -\frac{1}{2a^2}(t - t_0)^2 \right), \quad (38)$$

where $a = 0.015$, $t_0 = 1$. In this test, all fields are initially zero. We discretize the computational domain using the 4th-order SBP staggered grid operators and $201 \times 101$ grid points in the $(x_+, y_+)$ grid, such that $a/h = 3$. Figure 5 shows the pressure wave field at different snapshots in time. No spurious oscillations are visible.

To estimate the error, we compare the numerical solution to an analytic solution (see Appendix A). The absolute error in pressure is measured as
Figure 5: Snapshots in time of the pressure field due to a singular source term acting on the boundary. This test uses 200 × 100 grid points, $a/h = 3$, and the 4th-order staggered grid operators.
a function of time at the grid point in the center of the domain. Figure 6 shows that the numerical solution and semi-analytic solution are in excellent agreement. This test confirms that SBP staggered grid finite difference operators can handle singular source terms without producing any spurious oscillations.

![Figure 6: The error in the pressure obtained measured at the grid point in the center of the domain. (same as Figure 5)](image)

5.4. Multiblock interface treatment

In this final experiment, we showcase the multiblock capabilities of the SBP-SAT scheme by coupling subdomains with different material properties. We consider two subdomains located above and below the interface $x = 0$. Let $\bar{\Omega} = [0, 6] \times [0, 1]$ be the top subdomain and let $\Omega = [0, 6] \times [-2, 0]$ be the bottom subdomain. The wave speed $\bar{c}$ in $\bar{\Omega}$ is lower than the wave speed $c$ in $\Omega$. We use $c = 2\bar{c} = 2$ (constant). In each subdomain, we solve
the symmetrized, acoustic wave equation,

\begin{align*}
\frac{\partial \tilde{p}}{\partial t} + \tilde{c} \frac{\partial \tilde{u}}{\partial x} + \tilde{c} \frac{\partial \tilde{v}}{\partial y} &= 0, \\
\frac{\partial \tilde{u}}{\partial t} + \tilde{c} \frac{\partial \tilde{p}}{\partial x} &= 0, \\
\frac{\partial \tilde{v}}{\partial t} + \tilde{c} \frac{\partial \tilde{p}}{\partial y} &= 0, \quad (x, y) \in \tilde{\Omega}, \quad t \geq 0,
\end{align*}

\begin{align*}
\frac{\partial p}{\partial t} + c \frac{\partial u}{\partial x} + c \frac{\partial v}{\partial y} &= 0, \\
\frac{\partial u}{\partial t} + c \frac{\partial p}{\partial x} &= 0, \\
\frac{\partial v}{\partial t} + c \frac{\partial p}{\partial y} &= 0, \quad (x, y) \in \Omega, \quad t \geq 0.
\end{align*}

In (39), we have introduced the following symmetrization

\begin{align*}
p = \frac{\tilde{p}}{\sqrt{2K}}, \quad u = \sqrt{\frac{\rho}{2}} \tilde{u}, \quad v = \sqrt{\frac{\rho}{2}} \tilde{v},
\end{align*}

where $K > 0$ and $\rho > 0$ is the bulk modulus and density of the material, and $\tilde{p}, \ [\tilde{u}, \ \tilde{v}]^T$ are the unsymmetrized pressure and velocity field, respectively.

Since the wave speed is discontinuous across the interface, we discretize $\Omega$ and $\tilde{\Omega}$ using a multiblock discretization. The discretization is grid conforming, i.e., the grid points of each block along the interface are collocated. The two subdomains are coupled at the interface by enforcing

\begin{align*}
\tilde{p}(0, y, t) = \tilde{p}(0, y, t), \quad \tilde{u}(0, y, t) = \tilde{u}(0, y, t),
\end{align*}

see Appendix B for details on the SBP-SAT implementation. On the top boundary, we impose the free-surface boundary condition

\begin{align*}
p(x, 1, t) = 0.
\end{align*}

All fields are initialized to zero. To excite (or generate) waves, we add the following singular source term to (39),

\begin{align*}
\frac{\partial \tilde{p}}{\partial t} + \tilde{c} \frac{\partial \tilde{u}}{\partial x} + \tilde{c} \frac{\partial \tilde{v}}{\partial y} &= \delta(x - x_*)\delta(y - y_*)g(t).
\end{align*}

The source location is taken to be $(x_* = 3, \ y_* = 0.5)$ (located in the center of $\tilde{\Omega}$). The source time function is given by the Gaussian function

\begin{align*}
g(t) = \exp \left( -\frac{1}{2a^2} (t - t_0)^2 \right),
\end{align*}

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with \( a = 0.125 \) and \( t_0 = 6a \). We introduce the following parameters to establish how well-resolved the simulation is in each direction

\[
\bar{M}_x = \frac{a\bar{c}}{h_x} \quad \text{and} \quad \bar{M}_y = \frac{a\bar{c}}{h_y}, \quad (x, y) \in \bar{\Omega},
\]

\[
M_x = \frac{ac}{h_x} \quad \text{and} \quad M_y = \frac{ac}{h_y}, \quad (x, y) \in \bar{\Omega},
\]

where \( \bar{h} \) and \( h \) is the grid spacing in each subdomain, respectively.

In our first test, we use \( \bar{M} = 6 \) and \( M = 12 \), i.e., the grid spacing is uniform \((h_x = h_y = \bar{h}_x = \bar{h}_y)\). Figure 7 shows snapshots in time of the pressure field. In this simulation, waves from an explosion are reflected against the free surface and material interface. We have also solved this problem using a lower resolution \( \bar{M} = 3 \) and \( M = 6 \). Both simulations are in excellent agreement (cf. Figure 7c and Figure 8a).

We also compare the multiblock approach to a single-block-discretization. The single-block-discretization is inconsistent due to the material discontinuity. There is another disadvantage with the single-block-discretization. The subdomain \( \Omega \) is over-resolved because the grid resolution has been set by the accuracy requirements of \( \bar{\Omega} \), having the shortest wavelength. With the multiblock approach, we increase the grid spacing in the \( y \)-direction of \( \bar{\Omega} \) such that we have the same resolution \( \bar{M}_y = M_y \) in each subdomain. In this test, the modification reduces the computational cost by 35% without destroying the accuracy of the solution (Figure 8a). To confirm that we have not overresolved the solution, we also increase the grid spacing in the \( y \)-direction in \( \bar{\Omega} \). As expected, Figure 8b shows that this modification results in visible errors.

One can obtain a more significant improvement in computational efficiency by using non-conforming grids. Many methods have been proposed for interpolating across non-conforming, staggered grids, see e.g., \[20, 21, 22\] and the references therein. To the best of our knowledge, these methods are restricted to coarse-to-fine grid spacing ratios of integer order and have no proofs of stability. With SBP-SAT, provably stable interpolation methods have been developed for non-conforming, collocated grids \[23, 16\]. These methods should be directly applicable or straightforward to extend to staggered grids.
Figure 7: Snapshots in time of the pressure field. This test uses 4th-order SBP staggered grid operators on a multiblock grid. The grid resolution is $\bar{M} = 6$ and $M = 12$ ($768 \times 384$ grid points).
Figure 8: The pressure at time $t = 3$ in $\Omega$ (a) accurate resolution with constant resolution in the $y$-direction. (b) inaccurate result due to under-resolving the solution in the $y$-direction.
6. Conclusions

In this work, we extended the SBP-SAT approach to staggered grids. This extension combines the excellent dispersion properties of high-order accurate finite difference approximations on staggered grids with the excellent stability properties of the SBP-SAT approach. The key idea that made this extension possible was a new summation-by-parts property. This property, together with a weak enforcement of boundary conditions, enabled us to show stability by deriving a discrete energy estimate. Although we only considered the scalar wave equation, the method can likely be applied to e.g., the elastic wave equation, and various anisotropic scalar wave equations with minor modifications.

To assess the accuracy and showcase the capabilities of the method, we performed a series of numerical experiments. First, we showed convergence and demonstrated that the SBP staggered grid operators outperform the collocated SBP operators for wave propagation over large distances. Second, we ran a test with a singular source term on the boundary to confirm that the SBP boundary modification did not introduce any spurious oscillations. Finally, we applied an SBP-SAT multiblock discretization to solve a problem with a material discontinuity. We improved the computational efficiency compared to a single block discretization by reducing the number of grid points in the normal direction with respect to the interface of the block with the largest wave speeds. The multiblock capability of SBP-SAT schemes is a powerful tool that extends beyond the discretization of discontinuous material structures. For example, it can be used to couple non-conforming grids, unstructured and structured grids, as well as solving coupled multi-physics problems.

7. Acknowledgments

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Appendix A. Analytic solution of the singular source term problem

The solution to the problem in Section 5.3 can be obtained using Fourier transform methods [24, 25, 26]. The solution, obtained first in the frequency
domain, was then inverted to the time domain using an inverse Fast Fourier Transform (FFT).

Recall that the problem is given by solving the acoustic wave equation [18] in a half-space with the boundary condition

\[ p(x, 1, t) = g(t)\delta(x - x_*), \]

where \( g(t) \) is a known source time function.

The convention adopted for the Fourier transform is

\[ \hat{p}(x,y,\omega) = \int_{-\infty}^{\infty} p(x,y,t) e^{i\omega t} dt, \]

where \( i \) is the imaginary unit. In frequency domain, the solution to the problem is

\[ \hat{p}(x,y,\omega) = -\frac{|y - 1| H^{(1)}_1(z) \hat{g}(\omega)}{2cr}, \quad z = -\frac{\omega r}{c}, \quad r = \sqrt{(x - x_*)^2 + (y - 1)^2}. \]  

(A.1)

In (A.1), \( H^{(1)}_1(z) \) is the complex conjugate of the Bessel function of the third kind (Hankel function), \( r \) is radial distance of the source location to the observation point \((x,y)\), and \( c \) is the wave speed \((c = 1\) in Section 5.3\)), and \( \hat{g}(\omega) \) is the Fourier transform of the source time function \( g(t) \).

Appendix B. Multiblock coupling

In this section, we present a stable, multiblock coupling procedure using SBP-SAT. We only consider the one dimensional case, but the analysis can be extended to two dimensions by following the procedure laid out in Section 4.2.

Without loss of generality, we couple the left boundary to the right boundary of a single block (the multiblock coupling uses the same conditions). Consider the unsymmetrized wave equation with variable coefficients:

\[ \frac{1}{K} \frac{\partial \tilde{p}}{\partial t} + \frac{\partial \tilde{u}}{\partial x} = 0, \quad \rho \frac{\partial \tilde{u}}{\partial t} + \frac{\partial \tilde{p}}{\partial x} = 0. \]  

(B.1)

where \( K = K(x) \) is the bulk modulus, \( \rho = \rho(x) \) is the density, and \( c(x) = \sqrt{K/\rho} \) is the wave speed. The mechanical energy per unit area is

\[ E = \frac{1}{2} \int_0^1 \frac{\tilde{p}^2}{K} + \rho \tilde{u}^2 dx, \]

(B.2)
where the first term is the elastic energy and the second term is the kinetic energy. By taking the time derivative of (B.2) and using (B.1), results in

$$\frac{dE}{dt} = -\tilde{p}\tilde{u}|_{0}.$$  

The appropriate physical coupling conditions are obtained by requiring the pressure and normal velocity to be continuous at the interface:

$$\tilde{p}|_{0} = \tilde{p}|_{1} \quad \text{and} \quad \tilde{u}|_{0} = \tilde{u}|_{1}. \quad \text{(B.3)}$$

A semi-discrete approximation of (B.4) is written as

$$K^{-1}\frac{d\tilde{p}}{dt} + D\tilde{u} = P^{-1}_{N-}(\tilde{u}_{N} - \tilde{u}^{*}) - P^{-1}_{0-}(\tilde{u}_{0} - \tilde{u}^{*}),$$

$$\rho \frac{d\tilde{u}}{dt} + D\tilde{p} = P^{-1}_{N+}(\tilde{p}_{N} - \tilde{p}^{*}) - P^{-1}_{0+}(\tilde{p}_{0} - \tilde{p}^{*}), \quad \text{(B.4)}$$

where $K = \text{diag}([K_{0}, K_{1/2}, \ldots, K_{N-1/2}, K_{N}])$ and $\rho = \text{diag}([\rho_{0}, \rho_{1}, \ldots, \rho_{N}])$ holds the material properties at each grid point. The coupling conditions (B.3) are enforced by choosing the numerical fluxes $\tilde{p}^{*}$ and $\tilde{u}^{*}$. We use

$$\tilde{p}^{*} = \frac{\alpha\beta}{\alpha + \beta}(\tilde{u}_{N} - \tilde{u}_{0}) + \frac{\beta\tilde{p}_{0} + \alpha\tilde{p}_{N}}{\alpha + \beta} \quad \text{and} \quad \tilde{u}^{*} = \frac{\alpha\tilde{u}_{0} + \beta\tilde{u}_{N}}{\alpha + \beta} + \frac{\tilde{p}_{N} - \tilde{p}_{0}}{\alpha + \beta}. \quad \text{(B.5)}$$

where $\alpha$ and $\beta$ are the acoustic impedance of the medium on each side of the interface ($\alpha = \rho_{0}c_{0} > 0$ and $\beta = \rho_{N}c_{N} > 0$). This choice takes into account that the material properties $\rho$ and $K$ can be discontinuous across the interface. By using the SBP property (3), we can easily show stability. We have the following proposition.

**Proposition 3.** The semi-discrete approximation (B.4) of (B.1) using the numerical fluxes (B.5) is stable.

**Proof.** Analogous to the continuous energy (B.2), a discrete energy is defined as

$$E_{h} = \frac{1}{2}\tilde{p}^{T}K^{-1}P_{-}\tilde{p} + \frac{1}{2}\tilde{u}^{T}\rho P_{+}\tilde{u}. \quad \text{(B.6)}$$
By multiplying each equation in (B.4) by $\tilde{p}^TP_-$ and $\tilde{u}^TP_+$ from the left, and by using the SBP property (3), we get

$$
\frac{dE_h}{dt} = -\tilde{p}^T(Q_+ + Q_-^T)\tilde{u} + \tilde{p}_N(\tilde{u}_N - \tilde{u}^*) - \tilde{p}_0(\tilde{u}_0 - \tilde{u}^*)
+ \tilde{u}_N(\tilde{p}_N - \tilde{p}^*) - \tilde{u}_0(\tilde{p}_0 - \tilde{p}^*)
= \tilde{p}_0\tilde{u}_0 - \tilde{p}_N\tilde{u}_N + (\tilde{p}_0 - \tilde{p}_N)\tilde{u}^* + (\tilde{u}_0 - \tilde{u}_N)\tilde{p}^*. 
$$

Finally, by inserting (B.5) into (B.7), we get

$$
\frac{dE_h}{dt} = -\frac{1}{\alpha + \beta}(\tilde{p}_0 - \tilde{p}_N)^2 - \frac{\alpha\beta}{\alpha + \beta}(\tilde{u}_0 - \tilde{u}_N)^2 \leq 0. \quad \text{(B.8)}
$$

The result (B.8) shows that numerical dissipation is introduced in the scheme if $\alpha + \beta > 0$, and this dissipation vanishes with grid refinement as the numerical solution converges to the solution of the continuous problem.


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