

SUMMATION-BY-PARTS IN TIME: THE SECOND DERIVATIVE*

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Abstract. We analyze the extension of summation-by-parts operators and weak boundary conditions for solving initial boundary value problems involving second derivatives in time. A wide formulation is obtained by first rewriting the problem on first order form. This formulation leads to optimally sharp fully discrete energy estimates that are unconditionally stable and high order accurate. Furthermore, it provides a natural way to impose mixed boundary conditions of Robin type, including time and space derivatives. We apply the new formulation to the wave equation and derive optimal fully discrete energy estimates for general Robin boundary conditions, including nonreflecting ones. The scheme utilizes wide stencil operators in time, whereas the spatial operators can have both wide and compact stencils. Numerical calculations verify the stability and accuracy of the method. We also include a detailed discussion on the added complications when using compact operators in time and give an example showing that an energy estimate cannot be obtained using a standard second order accurate compact stencil.

Key words. time integration, second derivative approximation, initial value problem, high order accuracy, wave equation, second order form, initial boundary value problems, boundary conditions, stability, convergence, finite difference, summation-by-parts operators, weak initial conditions

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1. Introduction. Hyperbolic partial differential equations on second order form appear in many fields of applications, including electromagnetics, acoustics, and general relativity; see, for example, [1, 16] and references therein. The most common way of solving these equations has traditionally been to rewrite them on first order form and apply well-established methods for solving first order hyperbolic problems. For the time integration part, a popular choice due to its time reversibility is the leap-frog method, especially for long time simulations of wave propagation problems. This traditional approach does, however, have some disadvantages. Most notably it increases the number of unknowns and requires a higher resolution in both time and space [15]. Many attempts have been made to instead discretize the second order derivatives directly with finite difference approximations. Various types of compact difference schemes have been proposed, including, e.g., the classical Störmer and Numerov methods [10, 20, 12], as well as the Runge–Kutta-type one-step methods [10].

Of particular interest to us is the development of schemes based on high order accurate operators in space obeying a summation-by-parts (SBP) rule together with the weak simultaneous-approximation-term (SAT) penalty technique for boundary conditions [6, 14]. The SBP-SAT technique in space in combination with well-posed boundary conditions leads to energy stable semidiscrete schemes. By augmenting the SBP-SAT technique in space with SBP-SAT in time, we arrive at a procedure that leads in an almost automatic way to fully discrete schemes with unconditional stability. For a comprehensive review of the SBP-SAT technique, see [22]. Even

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though we focus on problems discretized by the SBP-SAT technique in space, we stress that the methodology is completely general and suitable for other types of semidiscrete energy stable spatial formulations.

In this paper we extend the SBP-SAT technique by using SBP operators also for the second derivative in time, leading to an implicit time stepping scheme. A similar technique was developed for first derivatives in [18, 13]. The main advantage of this approach is that it leads to optimal fully discrete energy estimates, guaranteeing unconditional stability and low dissipation. The schemes thus obtained can be in global or multistage form, or any combination of the two. A formulation using wide stencil second derivative operators can be obtained by first rewriting the equation in first order form and applying the SBP-SAT technique for first order initial value problems. The wide second derivative operator is obtained by operating twice with a first derivative operator. We show that the resulting discretizations work perfectly together with boundary conditions involving time derivatives and also lead to optimally sharp fully discrete energy estimates.

For problems formulated on an infinite time domain, i.e., where no boundaries are considered, we show that a stable scheme using compact stencils in time can be derived from combining two one-sided approximations of the first order formulation. Adding boundaries to the time domain with initial conditions, however, proves to be a difficult problem, and we find that the standard compact finite difference schemes are not appropriate for SBP-SAT discretizations of second time derivatives.

The organization of this paper is as follows. In section 2 we introduce the basic technique by demonstrating the SBP-SAT method applied to a first order initial value problem. We extend this in section 3, proposing an energy stable SBP-SAT implementation of second order problems. We obtain the discrete formulation by applying a first derivative SBP operator twice, thus resulting in a wide stencil scheme. In section 4 we apply the new method to the wave equation with general mixed Robin boundary conditions, demonstrating that it also leads to optimal fully discrete energy estimates. In section 5 we address the possibility of using a compact stencil formulation for the second derivative in time. Section 6 deals with the spectrum and existence of solutions for the first- and second order forms, respectively. Numerical calculations demonstrating the stability and accuracy of the newly developed method are presented in section 7. Finally, in section 8, conclusions are drawn.

2. First derivative approximations. We start by introducing the SBP-SAT technique for solving initial value problems of first order. A complete description of this time integration technique can be found in [18, 13]. Consider the scalar constant coefficient problem:

$$(1) \quad u_t + \lambda u = 0, \quad 0 \leq t \leq T,$$

where λ is a real constant. An energy estimate is obtained by multiplying (1) with u and then integrating over the domain. Assuming an initial value given by $u(0) = f$, we get

$$(2) \quad u(T)^2 + 2\lambda \|u\|_{L_2}^2 = f^2,$$

where the L_2 norm is defined as $\|u\|_{L_2}^2 = \int_0^T u^2 dt$.

The estimate (2) is the target for the numerical approximation. We introduce a discrete grid $\vec{t} = (0, \Delta t, \dots, T)$ with uniform spacing $\Delta t = T/N$ and a corresponding discrete solution $\vec{u} = (u_0, u_1, \dots, u_N)$. The discrete time derivative approximation is

obtained by using a finite difference first derivative operator in SBP form. We define

$$(3) \quad \vec{u}_t = D_1 \vec{u},$$

where the SBP property is given by

$$(4) \quad D_1 = P^{-1}Q, \quad Q + Q^T = B, \quad P = P^T > 0.$$

In (4), we have $B = \vec{e}_N \vec{e}_N^T - \vec{e}_0 \vec{e}_0^T$, where $\vec{e}_0 = (1, 0, \dots, 0)^T$ and $\vec{e}_N = (0, \dots, 0, 1)^T$. It now remains to impose the initial condition in a stable way by a penalty term.

The fully discrete approximation of (1) becomes

$$(5) \quad \vec{u}_t + \lambda \vec{u} = P^{-1} \tau (u_0 - f) \vec{e}_0.$$

We choose $\tau = -1$ and apply the energy method by multiplying (5) from the left with $\vec{u}^T P$ and then adding the transpose. This yields, after adding and subtracting f^2 ,

$$(6) \quad u_N^2 + 2\lambda \|\vec{u}\|_P^2 = f^2 - (u_0 - f)^2.$$

The discrete norm is defined as $\|\vec{u}\|_P^2 = \vec{u}^T P \vec{u}$, and the estimate (6) mimics the continuous target (2), only introducing a small additional damping term.

Although the SBP-SAT discretization above is presented for global finite difference operators in SBP form, we showed in [13] that the time interval can be divided into an arbitrary number of subdomains, allowing for a multistage formulation of the method that reduces the number of unknowns in each solution step. Other operators on SBP form, such as spectral element operators [5], can be used to reduce the number of unknowns even further. See also [7] for an overview of the possible ways to construct SBP operators, including a generalized approach. It should finally be noted that the resulting time integration schemes can in fact be shown to form a subset of implicit Runge–Kutta schemes [4].

3. Wide second derivative approximations. As a first test problem for treating second order derivatives in time, we extend the scalar constant coefficient case to the second order equation:

$$(7) \quad u_{tt} + \alpha^2 u_t + \beta^2 u = 0, \quad 0 \leq t \leq T,$$

where α^2 and β^2 are positive real constants. For this problem, an energy estimate is obtained by multiplying with u_t and then integrating over the domain. Given two initial conditions $u(0) = f$ and $u_t(0) = g$, the energy method yields the estimate

$$(8) \quad u_t(T)^2 + \beta^2 u(T)^2 + 2\alpha^2 \|u_t\|_{L_2}^2 = g^2 + \beta^2 f^2,$$

which is the target for our discrete energy estimate.

Since we multiply (7) with the time derivative of the solution, we can impose the second initial condition $u_t(0) = g$ in a stable way with the standard penalty technique used for the first order equation in (5). However, implementing the first initial condition $u(0) = f$ is more complicated and needs careful treatment. We start by transforming (7) into a system of first order differential equations. Setting $u_t = v$ and applying the SBP-SAT technique for first order systems as described in the previous section, we get

$$(9) \quad \begin{aligned} D_1 \vec{u} - \vec{v} &= P^{-1} \tau_0 (u_0 - f) \vec{e}_0, \\ D_1 \vec{v} + \alpha^2 \vec{v} + \beta^2 \vec{u} &= P^{-1} \tau_{0t} (v_0 - g) \vec{e}_0. \end{aligned}$$

We note that the first equation in (9) above can be used to define a modified discrete first derivative, with the weak SAT condition added to it. Indeed, we let $\tilde{u}_t = \vec{v}$, which gives

$$(10) \quad \tilde{u}_t = \vec{u}_t - P^{-1}\tau_0(u_0 - f)\vec{e}_0,$$

where $\vec{u}_t = D_1\vec{u}$ as in (3). Note also that the modified discrete first derivative \tilde{u}_t has the same order of accuracy as \vec{u}_t . Inserting (10) into the second equation in (9) leads to

$$(11) \quad \tilde{u}_{tt} + \alpha^2\tilde{u}_t + \beta^2\vec{u} = P^{-1}\tau_{0t}((\tilde{u}_0)_t - g)\vec{e}_0,$$

where the modified discrete second derivative is defined by applying the first derivative operator again on \tilde{u}_t :

$$(12) \quad \tilde{u}_{tt} = D_1\tilde{u}_t.$$

With the choice $\tau_0 = \tau_{0t} = -1$, the discrete energy method (multiplying (11) from the left with $\tilde{u}_t^T P$) now gives

$$(13) \quad ((\tilde{u}_N)_t)^2 + \beta^2 u_N^2 + 2\alpha^2 \|\tilde{u}_t\|_P^2 = h^2 + \beta^2 f^2 - ((\tilde{u}_0)_t - g)^2 - \beta^2 (u_0 - f)^2,$$

which is very similar to the continuous estimate (8).

We have proved the following.

PROPOSITION 1. *The approximation (11) with $\tau_0 = \tau_{0t} = -1$ and the modified first derivative (10) is an unconditionally stable approximation of the initial value problem (7) with the two initial conditions $u(0) = f$ and $u_t(0) = g$.*

Remark 2. Note that the additional complications that prompted the modified first derivative above are due to the initial value problem. If a boundary value problem had been considered with the conditions $u = f$, $u = g$ posed at different boundaries, the standard SBP-SAT technique could have been used. Note also that the choice $\tau_0 = \tau_{0t} = -1$ is a special choice that leads to the clean estimate (13). The approximation is stable for $\tau_0 \leq -1/2$ and $\tau_{0t} \leq -1/2$.

Remark 3. Note that in order to apply the discrete energy method, a clear separate definition of the first derivative is needed. This is straightforward as long as we use the wide operator D_1^2 to approximate the second derivative in the definition of \tilde{u}_{tt} in (12). The question arises whether an energy estimate can be obtained also for a compact formulation applied to an initial value problem. We will return to this question in section 5.

3.1. Multiblock/stage formulation. So far we have considered the application of the SBP-SAT technique to discretize second order problems in time as a global method; i.e., we solve (7) on the entire time interval of interest through a single fully coupled equation system. However, it is often advantageous to divide the problem into smaller time intervals, thus reducing the number of unknowns in each step. In this section we consider the two-block case. The extension to a fully multistage version is completely analogous.

Consider problem (7) divided into two time-slots

$$\begin{aligned} u_{tt} + \alpha^2 u_t + \beta^2 u &= 0, & 0 \leq t \leq t_i, \\ v_{tt} + \alpha^2 v_t + \beta^2 v &= 0, & t_i \leq t \leq T, \end{aligned}$$

with the same initial conditions as in the one domain formulation. We define the modified discrete first derivatives as

$$(14) \quad \begin{aligned} \tilde{u}_t &= D_1 \tilde{u} - P^{-1} \tau_L (u_N - v_0) \vec{e}_N - P^{-1} \tau_0 (u_0 - f) \vec{e}_0, \\ \tilde{v}_t &= D_1 \tilde{v} - P^{-1} \tau_R (v_0 - u_N) \vec{d}_0, \end{aligned}$$

where τ_L and τ_R are additional SAT penalty parameters forcing the solutions u_N and v_0 toward each other. The unit vectors \vec{e}_N and \vec{d}_0 both correspond to the time $t = t_i$. An SBP-SAT discretization of the two-block problem is

$$\begin{aligned} D_1 \tilde{u}_t + \alpha^2 \tilde{u}_t + \beta^2 \tilde{u} &= P^{-1} \tau_{Lt} ((\tilde{u}_N)_t - (\tilde{v}_0)_t) \vec{e}_N + P^{-1} \tau_{0t} ((\tilde{u}_0)_t - g) \vec{e}_0, \\ D_1 \tilde{v}_t + \alpha^2 \tilde{v}_t + \beta^2 \tilde{v} &= P^{-1} \tau_{Rt} ((\tilde{v}_0)_t - (\tilde{u}_N)_t) \vec{d}_0, \end{aligned}$$

where τ_{Lt} and τ_{Rt} force $(u_N)_t$ and $(v_0)_t$ toward each other. We set $\tau_0 = \tau_{0t} = -1$ as before.

The energy method now yields

$$\begin{aligned} \tilde{u}_t^T Q \tilde{u}_t + \alpha^2 \tilde{u}_t^T P \tilde{u}_t + \beta^2 \tilde{u}_t^T P \tilde{u} + \beta^2 u_0 (u_0 - f) - \beta^2 \tau_L u_N (u_N - v_0) \\ = \tau_{Lt} (\tilde{u}_N)_t ((\tilde{u}_N)_t - (\tilde{v}_0)_t) - (\tilde{u}_0)_t ((\tilde{u}_0)_t - g), \\ \tilde{v}_t^T Q \tilde{v}_t + \alpha^2 \tilde{v}_t^T P \tilde{v}_t + \beta^2 \tilde{v}_t^T P \tilde{v} - \beta^2 \tau_R v_0 (v_0 - u_N) \\ = \tau_{Rt} (\tilde{v}_0)_t ((\tilde{v}_0)_t - (\tilde{u}_N)_t), \end{aligned}$$

which can be rewritten as

$$\begin{aligned} ((\tilde{v}_t)_M)^2 + \beta^2 v_M^2 + 2\alpha^2 (\|\tilde{u}_t\|_P^2 + \|\tilde{v}_t\|_P^2) &= h^2 + \beta^2 f^2 - ((\tilde{u}_0)_t - g)^2 - \beta^2 (u_0 - f)^2 \\ &+ \beta^2 \begin{pmatrix} u_N \\ v_0 \end{pmatrix}^T \begin{pmatrix} -1 + 2\tau_L & -\tau_L - \tau_R \\ -\tau_L - \tau_R & 1 + 2\tau_R \end{pmatrix} \begin{pmatrix} u_N \\ v_0 \end{pmatrix} \\ &+ \begin{pmatrix} (\tilde{u}_N)_t \\ (\tilde{v}_0)_t \end{pmatrix}^T \begin{pmatrix} -1 + 2\tau_{Lt} & -\tau_{Lt} - \tau_{Rt} \\ -\tau_{Lt} - \tau_{Rt} & 1 + 2\tau_{Rt} \end{pmatrix} \begin{pmatrix} (\tilde{u}_N)_t \\ (\tilde{v}_0)_t \end{pmatrix}. \end{aligned}$$

A stable and conservative interface treatment requires that the following conditions must be fulfilled (for a proof, see [6]):

$$(15) \quad \tau_L = \tau_R + 1, \quad \tau_R \leq -\frac{1}{2}, \quad \tau_{Lt} = \tau_{Rt} + 1, \quad \tau_{Rt} \leq -\frac{1}{2}.$$

In particular, the choice $\tau_R = \tau_{Rt} = -1$ gives the sharp estimate

$$\begin{aligned} ((\tilde{v}_t)_M)^2 + \beta^2 v_M^2 + 2\alpha^2 (\|\tilde{u}_t\|_{P_L}^2 + \|\tilde{v}_t\|_{P_R}^2) &= g^2 + \beta^2 f^2 \\ &- ((\tilde{u}_0)_t - g)^2 - \beta^2 (u_0 - f)^2 \\ &- ((\tilde{u}_N)_t - (\tilde{v}_0)_t)^2 - \beta^2 (u_N - v_0)^2. \end{aligned}$$

Remark 4. The choice $\tau_R = \tau_{Rt} = -1$ also leads to $\tau_L = \tau_{Lt} = 0$ and hence makes the left domain completely uncoupled to the right one, enabling a multiblock/stage procedure.

By generalizing the derivation above we can prove the following.

PROPOSITION 5. *The multiblock/stage approximation of the initial value problem (7) with initial conditions $u(0) = f$ and $u_t(0) = g$ obtained by using (i) the penalty*

coefficients $\tau_0 = \tau_{0t} = -1$ for the initial conditions, (ii) modified first derivatives for the interface connection as in (14), and (iii) interface penalty coefficient as in (15) is an unconditionally stable approximation.

Remark 6. The multiblock/stage formulation introduces an extra amount of damping at each block boundary when compared to the global formulation for all stable penalty parameters, except for $\tau_R = \tau_{Rt} = -1/2$, where the damping is zero.

4. Space-time discretizations with mixed boundary conditions. The technique presented above for the test equation (7) extends in a natural way to general second order initial boundary value problems, including mixed boundary conditions with both time and space derivatives. To illustrate this, we consider the constant coefficient wave equation in one space dimension, with homogenous Robin boundary conditions:

$$(16) \quad \begin{aligned} u_{tt} &= \beta^2 u_{xx}, & 0 \leq x \leq 1, & 0 \leq t \leq T, \\ u(x, 0) &= f(x), \\ u_t(x, 0) &= g(x), \\ au_t(0, t) - u_x(0, t) &= 0, \\ au_t(1, t) + u_x(1, t) &= 0. \end{aligned}$$

The choice $a = 0$ corresponds to Neumann conditions, $a \rightarrow \infty$ to Dirichlet conditions, and $a = 1/\beta$ to nonreflecting artificial boundary conditions [8]. Even more general boundary conditions can also be considered [16].

To get an energy estimate for (16), we multiply with u_t and integrate in space. After accounting for the boundary conditions, we get

$$(17) \quad \frac{d}{dt} (\|u_t\|^2 + \beta^2 \|u_x\|^2) = -a\beta^2 (u_t(0, t)^2 + u_t(1, t)^2),$$

where $\|\cdot\|$ is the L_2 norm in space defined by $\|u\|^2 = \int_0^1 u^2 dt$. Thus, we have an energy estimate if $a > 0$. Finally, by time integration we obtain an estimate of the solution at the final time

$$(18) \quad \|u_t(\cdot, T)\|^2 + \|u_x(\cdot, T)\|^2 = \|g\|^2 + \|f_x\|^2 - a\beta^2 (\|u_t(0, \cdot)\|_{L_2}^2 + \|u_t(1, \cdot)\|_{L_2}^2),$$

where $\|\cdot\|_{L_2}$ as before is the L_2 norm in time.

4.1. The semidiscrete formulation. As the first step to approximate (16) we introduce a semidiscrete solution on the spatial grid $\vec{x} = (0, \Delta x, \dots, 1)$ with uniform spacing $\Delta x = 1/M$. We also define the restriction of the data f and h to this grid. Thus, let

$$\begin{aligned} \vec{u}(t) &= (u_0(t), u_1(t), \dots, u_M(t))^T, \\ \vec{f} &= (f(0), f(\Delta x), \dots, f(1))^T, \\ \vec{g} &= (g(0), g(\Delta x), \dots, g(1))^T. \end{aligned}$$

For convenience, we also introduce notation for the numerical derivatives of the solution and data vectors:

$$\vec{u}_x = D_x \vec{u}, \quad \vec{u}_{xx} = D_x \vec{u}_x, \quad \vec{f}_x = D_x \vec{f},$$

where $D_x = P_x^{-1}Q_x$ is an SBP operator; i.e., we have $Q_x + Q_x^T = B_x = \vec{e}_{Mx}\vec{e}_{Mx}^T - \vec{e}_{0x}\vec{e}_{0x}^T$, where $\vec{e}_{0x} = (1, 0, \dots, 0)^T$ and $\vec{e}_{Mx} = (0, \dots, 0, 1)^T$, in analogy with (14).

For future reference we also introduce the traditional compact second order derivatives in space which have the form

$$(19) \quad \vec{u}_{xx} = D_2\vec{u} = P^{-1}(-M + BS)\vec{u},$$

where $M + M^T \geq 0$, and S approximates the first derivative at the boundaries.

Remark 7. In the rest of the paper, the notation D_1, D_x, D_t is interchangeably used for the SBP operator approximating the first derivative. The subscripts indicate a general coordinate direction, the x -direction and the t -direction, respectively. The wide second derivate is denoted D_1^2 and the compact second derivative D_2 .

The SBP-SAT method in space now yields

$$(20) \quad \begin{aligned} \vec{u}_{tt} &= \beta^2\vec{u}_{xx} + P_x^{-1}\sigma_0(a(\vec{u}_t)_0 - (\vec{u}_x)_0)\vec{e}_{0x} \\ &\quad + P_x^{-1}\sigma_M(a(\vec{u}_t)_M + (\vec{u}_x)_M)\vec{e}_{0x}, \\ \vec{u}(x, 0) &= \vec{f}, \\ \vec{u}_t(x, 0) &= \vec{g}. \end{aligned}$$

Note that we have used the wide stencil operator D_x^2 for convenience to approximate the second spatial derivative. The extension to compact stencil operators in space of the form (19) poses no problem [16].

Multiplying (20) from the left with $\vec{u}_t^T P_x$ gives

$$\begin{aligned} \vec{u}_t^T P_x \vec{u}_{tt} &= \beta^2 \vec{u}_t^T Q_x \vec{u}_x + \sigma_0 (\vec{u}_t)_0 (a(\vec{u}_t)_0 - (\vec{u}_x)_0) + \sigma_M (\vec{u}_t)_M (a(\vec{u}_t)_M + (\vec{u}_x)_M) \\ &= -\beta^2 (D_x \vec{u}_t)^T P_x \vec{u}_x + a(\sigma_0 (\vec{u}_t)_0 + \sigma_M (\vec{u}_t)_M) \\ &\quad + (\beta^2 + \sigma_M)(u_t)_M (u_x)_M - (\beta^2 + \sigma_0)(u_t)_0 (u_x)_0, \end{aligned}$$

where we have used the SBP property $Q_x = B_x - Q_x^T$. Note that, since the time derivative is left continuous, we can change the order of differentiation in the first term of the right-hand side above as

$$(21) \quad -\beta^2 (D_x \vec{u}_t)^T P_x \vec{u}_x = -\beta^2 (\vec{u}_x)_t^T P_x \vec{u}_x = -\frac{\beta^2}{2} \frac{d}{dt} \|\vec{u}_x\|_{P_x}.$$

The choice $\sigma_0 = \sigma_M = -\beta^2$ now leads to

$$(22) \quad \frac{d}{dt} (\|\vec{u}_t\|_{P_x} + \beta^2 \|\vec{u}_x\|_{P_x}) = -a\beta^2 ((\vec{u}_t)_0^2 + (\vec{u}_t)_M^2).$$

Note that the relation (22) is completely analogous to the continuous (17). Finally, integrating in time yields

$$(23) \quad \begin{aligned} \|\vec{u}_t(T)\|_{P_x} + \beta^2 \|\vec{u}_x(T)\|_{P_x} &= \|\vec{g}\|_{P_x} + \beta^2 \|\vec{f}_x\|_{P_x} \\ &\quad - a\beta^2 \int_0^T (\|(\vec{u}_t)_0\|_{L_2}^2 + \|(\vec{u}_t)_M\|_{L_2}^2) dt, \end{aligned}$$

which mimics (18).

Remark 8. The wide second derivative approximation in (20) can be replaced with a compact approximation of the form (19). The estimate for the compact operator corresponding to (23) becomes

$$\begin{aligned} \vec{u}_t(T)^T P_x \vec{u}_t(T) + \beta^2 \vec{u}(T)^T M_x \vec{u}(T) &= \vec{g}^T P_x \vec{g} + \beta^2 \vec{f}^T M_x \vec{f} \\ &\quad - a\beta^2 \int_0^T ((u_t^2)_0 + (u_t^2)_M) dt. \end{aligned}$$

In other words, no problems occur, which is contrary to the case with compact operators in time, as will be discussed later.

4.2. The fully discrete formulation. Next, we introduce the fully discrete solution vector \vec{U} together with the corresponding numerical derivatives with respect to time and space:

$$\vec{U}_t = (D_t \otimes I_x) \vec{U}, \quad \vec{U}_x = (I_t \otimes D_x) \vec{U}, \quad \vec{U}_{xx} = (I_t \otimes D_x) \vec{U}_x,$$

where $D_t = P_t^{-1} Q_t$ and $D_x = P_x^{-1} Q_x$ as before are SBP operators, and I_t and I_x are unit matrices of dimensions $N + 1$ and $M + 1$, respectively. In direct analogy with (9), (10), and (12), we also define modified time derivatives with the first initial condition built in:

$$(24) \quad \tilde{\vec{U}}_t = \vec{U}_t - (P_t \otimes P_x)^{-1} T_0, \quad \tilde{\vec{U}}_{tt} = (D_t \otimes I_x) \tilde{\vec{U}}_t.$$

The penalty term in (24) is given by $T_0 = \tau_0(I_t \otimes P_x)(\vec{e}_{0t} \otimes (\vec{U}|_{t=0} - \vec{f}))$, where $\vec{U}|_{t=0} = (\vec{e}_{0t}^T \otimes I_x) \vec{U}$ is the solution at the first grid point in time.

The fully discrete SBP-SAT approximation of (16) can now be written as

$$(25) \quad \tilde{\vec{U}}_{tt} = \beta^2 \vec{U}_{xx} + (P_t \otimes P_x)^{-1} (T_{0t} + \Sigma),$$

where the initial and boundary conditions are imposed by

$$(26) \quad \begin{aligned} T_{0t} &= \tau_{0t}(I_t \otimes P_x)(\vec{e}_{0t} \otimes (\tilde{\vec{U}}_t|_{t=0} - \vec{g})), \\ \Sigma &= \sigma_0(P_t \otimes I_x)((a\tilde{\vec{U}}_t|_{x=0} - \vec{U}_x|_{x=0}) \otimes \vec{e}_{0x}) \\ &\quad + \sigma_M(P_t \otimes I_x)((a\tilde{\vec{U}}_t|_{x=1} + \vec{U}_x|_{x=1}) \otimes \vec{e}_{Mx}). \end{aligned}$$

In (24) and (26), we have used

$$\begin{aligned} \vec{U}|_{t=0} &= (\vec{e}_{0t}^T \otimes I_x) \vec{U}, & \tilde{\vec{U}}_t|_{t=0} &= (\vec{e}_{0t}^T \otimes I_x) \tilde{\vec{U}}_t, \\ \tilde{\vec{U}}_t|_{x=0} &= (I_t \otimes \vec{e}_{0x}^T) \tilde{\vec{U}}_t, & \tilde{\vec{U}}_t|_{x=1} &= (I_t \otimes \vec{e}_{Mx}^T) \tilde{\vec{U}}_t, \\ \vec{U}_x|_{x=0} &= (I_t \otimes \vec{e}_{0x}^T) \vec{U}_x, & \vec{U}_x|_{x=1} &= (I_t \otimes \vec{e}_{Mx}^T) \vec{U}_x \end{aligned}$$

to identify the solution components on the boundaries of the computational domain.

The fully discrete energy estimate is obtained by first multiplying (25) from the left with $\tilde{\vec{U}}_t^T (P_t \otimes P_x)$, which yields

$$\tilde{\vec{U}}_t^T (Q_t \otimes P_x) \tilde{\vec{U}}_t = \beta^2 \tilde{\vec{U}}_t^T (P_t \otimes Q_x) \vec{U}_x + \tilde{\vec{U}}_t^T (T_{0t} + \Sigma).$$

The SBP property of Q_t and Q_x now leads to

$$\begin{aligned}
 \frac{1}{2} \tilde{U}_t^T (B_t \otimes P_x) \tilde{U}_t &= \beta^2 \tilde{U}_t^T (P_t \otimes (B_x - Q_x^T)) \vec{U}_x + \tilde{U}_t^T (T_{0t} + \Sigma) \\
 (27) \qquad \qquad \qquad &= \beta^2 \tilde{U}_t^T (P_t \otimes B_x) \vec{U}_x - \beta^2 ((I_t \otimes D_x) \tilde{U}_t)^T (P_t \otimes P_x) \vec{U}_x \\
 &\quad + \tilde{U}_t^T (T_{0t} + \Sigma).
 \end{aligned}$$

Next, we rewrite the second term on the right-hand side of (27) above by changing the order of numerical differentiation, using the commutivity of the Kronecker products and the SBP property. We get, in analogy with the technique used for integrating (21) in time,

$$\begin{aligned}
 & - \beta^2 ((I_t \otimes D_x) \tilde{U}_t)^T (P_t \otimes P_x) \vec{U}_x \\
 (28) \quad &= - \beta^2 ((Q_t \otimes D_x) \vec{U})^T (I_t \otimes P_x) \vec{U}_x + \beta^2 \tau_0 e_{0t} \otimes (D_x (\vec{U}|_{t=0} - \vec{f}))^T (I_t \otimes P_x) \vec{U}_x \\
 &= - \frac{1}{2} \vec{U}_x^T (B_t \otimes P_x) \vec{U}_x + \beta^2 \tau_0 (U_x|_{t=0} - \vec{f}_x)^T P_x \vec{U}_x|_{t=0}.
 \end{aligned}$$

Moreover, the penalty terms in (27) simplify by (26) to

$$\begin{aligned}
 (29) \qquad \qquad \qquad & \tilde{U}_t^T T_{0t} = \tau_{0t} \tilde{U}_t|_{t=0}^T P_x (\tilde{U}_t|_{t=0} - \vec{g}), \\
 (30) \qquad \qquad \qquad & \tilde{U}_t^T \Sigma = \sigma_0 \tilde{U}_t|_{x=0}^T P_t (a \tilde{U}_t|_{x=0} - \vec{U}_x|_{x=0}) \\
 & \quad + \sigma_M \tilde{U}_t|_{x=1}^T P_t (a \tilde{U}_t|_{x=1} + \vec{U}_x|_{x=1}).
 \end{aligned}$$

Inserting (28)–(30) into (27) now gives

$$\begin{aligned}
 \tilde{U}_t|_{t=T}^T P_x \tilde{U}_t|_{t=T} + \beta^2 \vec{U}_x|_{t=T}^T P_x \vec{U}_x|_{t=T} &= \tilde{U}_t|_{t=0}^T P_x \tilde{U}_t|_{t=0} + \beta^2 \vec{U}_x|_{t=1}^T P_x \vec{U}_x|_{t=0} \\
 & \quad - 2(\beta^2 + \sigma_0) \tilde{U}_t|_{x=0}^T P_t \vec{U}_x|_{x=0} \\
 & \quad + 2(\beta^2 + \sigma_M) \tilde{U}_t|_{x=1}^T P_t \vec{U}_x|_{x=1} \\
 & \quad + 2a(\sigma_0 \tilde{U}_t|_{x=0}^T P_t | \tilde{U}_t|_{x=0} + \sigma_M \tilde{U}_t|_{x=1}^T P_t | \tilde{U}_t|_{x=1}) \\
 & \quad + 2\beta^2 \tau_0 (\vec{U}_x|_{t=0} - \vec{f}_x)^T P_x \vec{U}_x|_{t=0} \\
 & \quad + 2\tau_{0t} \tilde{U}_t|_{t=0}^T P_x (\tilde{U}_t|_{t=0} - \vec{g}).
 \end{aligned}$$

Finally, by choosing the penalty parameters as $\tau_0 = \tau_{0t} = -1$ and $\sigma_0 = \sigma_M = -\beta^2$, we arrive at the estimate

$$\begin{aligned}
 \tilde{U}_t|_{t=T}^T P_x \tilde{U}_t|_{t=T} + \beta^2 \vec{U}_x|_{t=T}^T P_x \vec{U}_x|_{t=T} &= \vec{g}^T P_x \vec{g} + \beta^2 \vec{f}_x^T P_x \vec{f}_x \\
 (31) \qquad \qquad \qquad & \quad - a\beta^2 (\tilde{U}_t|_{x=0}^T P_t | \tilde{U}_t|_{x=0} + \tilde{U}_t|_{x=1}^T P_t | \tilde{U}_t|_{x=1}) \\
 & \quad - (\tilde{U}_t|_{t=0} - \vec{g})^T P_x (\tilde{U}_t|_{t=0} - \vec{g}) \\
 & \quad - \beta^2 (\vec{U}_x|_{t=0} - \vec{f}_x)^T P_x (\vec{U}_x|_{t=0} - \vec{f}_x),
 \end{aligned}$$

which mimics both the continuous estimate (18) and the semidiscrete energy estimate (23).

We have proved the following.

PROPOSITION 9. *The fully discrete approximation (25) of (16) with initial and boundary conditions imposed by (26) and penalty coefficients $\tau_0 = \tau_{0t} = -1$, $\sigma_0 = \sigma_M = -\beta^2$ is unconditionally stable.*

Remark 10. By replacing the wide second derivative in space with a compact approximation of the form (19), we get the following estimate:

$$\begin{aligned} \tilde{U}_t|_{t=T}^T P_x \tilde{U}_t|_{t=T} + \beta^2 \tilde{U}|_{t=T}^T M_x \tilde{U}|_{t=T} &= \tilde{g}^T P_x \tilde{g} + \beta^2 \tilde{f}^T M_x \tilde{f} \\ &\quad - a\beta^2 (\tilde{U}_t|_{x=0}^T P_t \tilde{U}_t|_{x=0} + \tilde{U}_t|_{x=1}^T P_t \tilde{U}_t|_{x=1}) \\ &\quad - (\tilde{U}_t|_{t=0} - \tilde{g})^T P_x (\tilde{U}_t|_{t=0} - \tilde{g}) \\ &\quad - \beta^2 (\tilde{U}|_{t=0} - \tilde{f})^T M_x (\tilde{U}|_{t=0} - \tilde{f}), \end{aligned}$$

which corresponds to (31). Again, no complications occur, unlike the case with compact operators in time that will be discussed next.

Remark 11. Proposition 9 opens up the possibility for using more general non-reflecting boundary conditions (which typically contain time derivatives) and prove stability by using the energy method. Normally one has to use normal mode analysis, which is significantly more complicated and essentially limited to one-dimensional problems; see [8, 9].

5. Compact second derivative approximations. The wide second derivative approximations discussed so far in this paper have been derived through a first order reformulation of the problem. In this section we investigate the implications of extending the technique to compact formulations of the second derivative.

5.1. An infinite domain formulation. We begin by considering the test problem (1) on an unbounded interval, ignoring any influence from boundaries of the computational domain. Using one-sided difference operators D_+ and D_- instead of the central scheme used in (9) leads to one of the following two compact schemes:

$$(32) \quad D_+ D_- \bar{u} + \alpha^2 D_- \bar{u} + \beta^2 \bar{u} = 0,$$

$$(33) \quad D_- D_+ \bar{u} + \alpha^2 D_+ \bar{u} + \beta^2 \bar{u} = 0,$$

where $D_+ D_- = D_- D_+$ is a symmetric and compact second derivative difference scheme. The energy method applied directly on either (32) or (33) results in at least one term with positive sign in the right-hand side, since D_+ and D_- have elements with opposite signs along the diagonal. Instead we combine (32) and (33) into the following modified equation:

$$(34) \quad D_+ D_- \bar{u} + \alpha^2 D_0 \bar{u} + \beta^2 \bar{u} = 0,$$

where $D_0 = (D_- + D_+)/2$ is a central difference approximation. Note that the compact operator in (34) remains unchanged. The energy method (multiplying (34) with the central first derivative $(D_0 \bar{u})^T$ from the left) now yields

$$(35) \quad \bar{u}^T (D_0^T D_+ D_-) \bar{u} + \alpha^2 (D_0 \bar{u})^T (D_0 \bar{u}) + \beta^2 \bar{u}^T D_0 \bar{u} = 0.$$

To conclude that the scheme is stable, we first need the following lemma.

LEMMA 12. *Let A and B be two infinite matrices both consisting of a constant finite length interior stencil centered around the main diagonal. Then A and B commute, i.e., $AB = BA$.*

Proof. See Appendix A. □

Adding the transpose to (35) now gives

$$(36) \quad \vec{u}^T (D_0^T D_+ D_- + D_+ D_- D_0) \vec{u} + 2\alpha^2 (D_0 \vec{u})^T (D_0 \vec{u}) + \beta^2 \vec{u}^T (D_0 + D_0^T) \vec{u} = 0.$$

We first note that $D_0 + D_0^T = 0$, since the central difference scheme is skew-symmetric. Moreover, since D_0 and $D_+ D_-$ are both infinite matrices with constant diagonals, we get from Lemma 12 that $D_0^T D_+ D_- + D_+ D_- D_0 = D_0^T D_+ D_- + D_0 D_+ D_- = (-D_0 + D_0) D_+ D_- = 0$. Consequently, the only remaining part of (36) is

$$(37) \quad 2\alpha^2 (D_0 \vec{u})^T (D_0 \vec{u}) = 0,$$

which mimics (8), except for the boundary terms that we do not consider here. This technique for constructing a compact approximation thus works perfectly in the interior of a time domain. However, adding weak initial conditions will introduce difficulties that are hard, possibly even impossible, to overcome.

5.2. Compact summation-by-parts operators. We start this section with a short review of the construction of compact second derivative operators for space approximations with the SBP-SAT technique. Getting an energy estimate in these applications requires operators that mimic the following integral property of the continuous derivative:

$$(38) \quad \int_a^b uu_{xx} dx = u(b)u_x(b) - u(a)u_x(a) - \int_a^b u_x^2 dx.$$

For wide second derivative approximations defined by $\vec{u}_x = D_1 \vec{u}$ and $\vec{u}_{xx} = D_1 \vec{u}_x$, where D_1 is an SBP first derivative operator, a discrete counterpart of (38) follows directly:

$$\vec{u}^T P \vec{u}_{xx} = \vec{u}^T Q \vec{u}_x = \vec{u}^T (B - Q^T) \vec{u}_x = u_N(u_x)_N - u_0(u_x)_0 - \vec{u}_x^T P \vec{u}_x,$$

which corresponds to (38).

For the compact second operators of the form (19) we get

$$\vec{u}^T P \vec{u}_{xx} = \vec{u}^T B(S\vec{u}) - \frac{1}{2} \vec{u}^T (M + M^T) \vec{u},$$

which mimics (38) in the sense that we get an approximation of the boundary terms along with a damping term, leading to stability. An even closer similarity to (38) is obtained with so-called *compatible* operators, defined by $M = D_1^T P D_1 + R$, where $R + R^T \geq 0$ is a small additional damping term, giving

$$\vec{u}^T P \vec{u}_{xx} = \vec{u}^T B(S\vec{u}) - (D_1 \vec{u})^T P (D_1 \vec{u}) - \frac{1}{2} \vec{u}^T (R + R^T) \vec{u}.$$

Such compatible operators are in particular needed for problems with combinations of mixed and pure second derivatives, for which they were originally developed [17, 14]. Note that the wide operator D_1^2 corresponds to the compatible form with zero additional damping, $S = D_1$, and $D_1^2 = P^{-1}(-Q^T D_1 + B D_1) = P^{-1}(-D_1^T P D_1 + B D_1)$.

In contrast to (38) required for second order space approximations, we instead need to approximate the following integral identity:

$$(39) \quad \int_0^T u_t u_{tt} dt = \frac{1}{2} (u_t(T)^2 - u_t(0)^2)$$

for second order time approximations. Using the wide stencil approximation $\vec{u}_{tt} = D_1 \vec{u}_t$, where $\vec{u}_t = D_1 \vec{u}$, we get the following discrete estimate:

$$\vec{u}_t^T P \vec{u}_{tt} = \vec{u}_t^T Q \vec{u}_t = \frac{1}{2} \vec{u}_t^T B \vec{u}_t,$$

which mimics (39).

The standard compact definition $\vec{u}_{tt} = D_2 \vec{u}$, where D_2 is defined in (19), does, however, not automatically lead to an estimate. Assuming $S = D_1$, we get

$$(40) \quad \vec{u}_t^T P \vec{u}_{tt} = \frac{1}{2} \vec{u}_t^T B \vec{u}_t + \frac{1}{2} \vec{u}_t^T (-D_1^T M - M^T D_1 + D_1^T B D_1) \vec{u},$$

where $\vec{u}_t^T (-D_1^T M - M^T D_1 + D_1^T B D_1) \vec{u}$ is an indefinite term even if $M + M^T \geq 0$. The compatible form $M = D_1^T P D_1 + R$ does not improve the situation but leads to a simpler expression than (40). Indeed, we get

$$\vec{u}_t^T P \vec{u}_{tt} = \frac{1}{2} \vec{u}_t^T B \vec{u}_t - \vec{u}^T (D_1^T R + R^T D_1) \vec{u},$$

which requires $D_1^T R + R^T D_1$ to be a negative semidefinite matrix, since the second derivative u_{tt} resides on the left-hand side of the original equation.

To summarize, we get an estimate that mimics (39) with additional damping if the discrete second derivative can be written on the following form:

$$(41) \quad \vec{u}_{tt} = D_2 \vec{u} = D_1 \vec{u}_t - P^{-1} R \vec{u},$$

where $D_2 = P^{-1} (-D_1^T P D_1 - R + B D_1) = D_1^2 - P^{-1} R$, and where $D_1^T R + R^T D_1$ is a negative semidefinite matrix. Except for a rather extreme single example (shown in Appendix B), we have not yet been able to construct any other operator for which $D_1^T R + R^T D_1 \geq 0$. Furthermore, even if this could be done, the imposition of the weak initial conditions introduces additional complications that we believe are impossible to overcome. We discuss this in detail in Appendix B.

6. Spectrum and existence of solutions. The first and second order formulations lead to different matrix properties of the fully discretized system. That will be investigated next.

6.1. The initial value problem. We let $\tilde{D}_1 = D_1 + \vec{e}_0 \vec{e}_0^T$ denote a discrete first derivative operator augmented with a boundary correction of the optimal magnitude (corresponding to the choices $\tau, \tau_0, \tau_{0t} = -1$ in sections 2 and 3). Although a proof only exists for the second order accurate case, there are strong reasons to assert that the spectrum of \tilde{D}_1 lies strictly in the right half-plane for all classical SBP operators (see Assumption 1 in [18]).

The system matrix of the discretized initial value problem on first order form (9) can now be written as

$$A_1 = \begin{pmatrix} \tilde{D}_1 & -I \\ \beta^2 I & \tilde{D}_1 \end{pmatrix},$$

where we for simplicity let $\alpha^2 = 0$. Let $\lambda = a + bi$ be an eigenvalue to \tilde{D}_1 with corresponding eigenvector $\phi = x + iy$, i.e.,

$$\tilde{D}_1 x = ax - by, \quad \tilde{D}_1 y = bx + ay.$$

It follows that $\lambda + i\beta$ and $\lambda - i\beta$ are eigenvalues to A_1 , with eigenvectors given by $[x + iy, \beta(y - ix)]^T$ and $[y - ix, \beta(x + iy)]^T$, respectively. Indeed, multiplying A_1 from the right with the vector $[x + iy, \beta(y - ix)]^T$ leads to

$$A_1 \begin{pmatrix} x + iy \\ \beta(y - ix) \end{pmatrix} = \begin{pmatrix} ax - by + i(bx + ay) - \beta(y - ix) \\ \beta^2(x + iy) + \beta(bx + ay - i(ax - by)) \end{pmatrix} = (\lambda + i\beta) \begin{pmatrix} x + iy \\ \beta(y - ix) \end{pmatrix}.$$

We can verify that $\lambda - i\beta$ is an eigenvalue in the same way. This shows that the eigenvalues of A_1 have the same real parts as those of \tilde{D}_1 , which we already know are strictly positive. Thus the symmetric part of A_1 is positive definite, and as a consequence the matrix is also invertible.

The system matrix for the discretized initial value problem on second order form (11) can be expressed as

$$A_2 = (\tilde{D}_1^2 + \beta^2 I).$$

Thus A_2 share the same eigenvectors as \tilde{D}_1^2 , and the eigenvalues are given by $\lambda^2 + \beta^2$. Since the spectrum of \tilde{D}_1 is dominantly imaginary (see, e.g., Figure 1 in [18]), the spectrum of A_2 will be dominantly real, and with both positive and negative real parts unless the parameter β^2 is very large. However, most importantly, there are no zero eigenvalues to A_2 , since λ is never purely imaginary.

As we have seen, the spectrum associated with the first and the second order forms of the time discretization becomes rather different. In the first order formulation, the system is highly nonsymmetric with large imaginary parts of eigenvalues, whereas for the second order formulation the eigenvalues are dominantly real but indefinite. As we shall see, these same attributes are shared by the corresponding formulations of the fully discrete wave equation.

6.2. The wave equation. For the wave equation (16), we obtain the following system matrix by using the first order in time formulation of the fully discrete SBP-SAT discretization:

$$A_1 = \begin{pmatrix} \tilde{D}_t \otimes I_x & I_t \otimes I_x \\ -I_t \otimes \tilde{D}_{2x} & \tilde{D}_t \otimes I_x + I_t \otimes a\beta^2 P_x^{-1} (\vec{e}_{0x} \vec{e}_{0x}^T + \vec{e}_{Mx} \vec{e}_{Mx}^T) \end{pmatrix},$$

where $\tilde{D}_t = D_t + P_t^{-1} e_{0t} \vec{e}_{0t}^T$, and $\tilde{D}_{2x} = D_x(D_x - P^{-1} B_x)$. Note that D_{2x} is similar to $\sqrt{P_x} \tilde{D}_{2x} \sqrt{P_x}^{-1} = -\sqrt{P_x}^{-1} Q_x P_x^{-1} Q_x^T \sqrt{P_x}^{-1}$, which is a symmetric and negative semidefinite matrix. Thus the eigenvalues of \tilde{D}_{2x} are real and nonpositive.

For the special case of Neumann boundary conditions ($a = 0$), we can now easily extend the theory from the previous section to the current setting. Indeed, we consider an eigenvalue $\lambda = a + ib$ to \tilde{D}_t with eigenvector $\phi = x + iy$, as well as another eigenvalue $-\xi^2$ to \tilde{D}_{2x} with eigenvector ψ . It follows that the two vectors $[(x + iy) \otimes \psi, \beta\xi(y - ix) \otimes \psi]^T$ and $[(y - ix) \otimes \psi, \beta\xi(x + iy) \otimes \psi]^T$ are eigenvectors to A_1 if $a = 0$, with eigenvalues given by $\lambda + i\beta\xi$ and $\lambda - i\beta\xi$, respectively. This can be verified completely analogously as for the initial value problem.

The system matrix appearing in the fully discrete SBP-SAT approximation on second order form (25) can be written as

$$A_2 = \tilde{D}_t^2 \otimes I_x - I_t \otimes \beta^2 \tilde{D}_{2x} + \tilde{D}_t \otimes (a\beta^2 P_x^{-1} (\vec{e}_{0x} \vec{e}_{0x}^T + \vec{e}_{Mx} \vec{e}_{Mx}^T)).$$

Again, for Neumann conditions ($a = 0$) it is easy to extend the result obtained for the initial value problem in the previous section. In this case A_2 becomes the

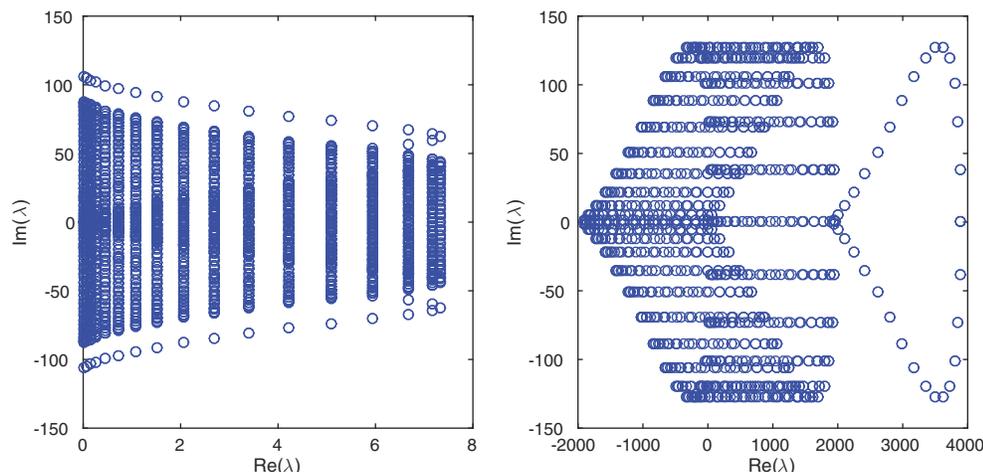


FIG. 1. Spectrum of the first (left) and second (right) order formulations of the fully discrete wave equation, using second order accurate SBP operators with $N_t = N_x = 32$.

Kronecker sum between the matrices \tilde{D}_t^2 and $-\beta^2 \tilde{D}_{2x}$. The eigenvalues are thus given by $\lambda^2 + \beta^2 \xi^2$, which in general is an indefinite, although nonzero, expression.

We illustrate the different spectrums obtained using the first and second order formulations in Figure 1, where we discretize the wave equation using second order accurate SBP operators (with first order accurate boundary closures). As expected, the spectrum is dominated by the imaginary part in the first order formulation, whereas in the second order formulation, the system is indefinite.

Finally, we note that also the condition numbers of the two matrices A_1 and A_2 differ considerably. In the example illustrated in Figure 1, for example, the condition numbers are $6.65 \cdot 10^6$ and $5.00 \cdot 10^3$, respectively.

7. Numerical calculations. In this section we consider fully discrete approximations of the one- and two-dimensional wave equations.

7.1. Accuracy. Consider a first derivative operator D_1 of order τ at the boundaries and $2s$ in the interior. (We refer to this operator and the resulting schemes as SBP($2s, \tau$).) By applying this operator twice, the boundary accuracy of the resulting wide stencil second order operator $D_2 = D_1^2$ is reduced to $\tau - 1$. From the theory in [21] we should thus expect the global order of convergence in time to be $\tau + 1$.

However, since the wide formulations (11) and (25) can be derived from solving the system on first order form in time, the theory for dual consistent formulations of first order systems also applies [13, 11, 2, 3]. A dual consistent scheme is obtained by the same choice of penalty parameters that lead to sharp energy estimates in (13) and (23), and this leads to superconvergence of order $2s$ for the solution at the final time step, as well as for other functionals of the solution.

We consider approximations to the wave equation (16) with wave speed $\beta^2 = 1$, employing the exact manufactured solution $u = \sin(2\pi t)\cos(2\pi x)$, providing initial data and boundary data for homogeneous Neumann boundary conditions. We use a very accurate discretization in space (SBP(8,7) with $M = 256$) to minimize the

spatial error component, and we apply the SBP-SAT discretization technique (25) using seven different operators in time. For diagonal norm operators we have $\tau = s$, and for block norms $\tau = 2s - 1$.

As we can see in Figure 2, the convergence rate is the expected $2s$ for all these operators. In Figure 3 we show the same results for a multistage implementation. We have used $N_i = 2, 8, 12$, and 16 in each stage for operators with internal order $2s = 2, 4, 6$, and 8 , respectively. Clearly, there is no drop in accuracy compared with the global approach.

7.2. A comparison with other methods. We make an initial comparison of the performance between the SBP-SAT technique and a few other unconditionally stable methods for ordinary differential equations on second order form.

The classical fully implicit Runge–Kutta schemes based on Gauss–Lobatto quadrature share many of the same characteristics of the classical SBP-SAT technique with diagonal norms, including order ($2s$, with stage order s) and stability (A -stability, L -stability, and B -stability). One can even show that they are a particular form of the SBP-SAT schemes with diagonal norm; see [4]. When applied to second order problems, this leads to the so-called indirect Runge–Kutta–Nyström approach [10, 23] with $s + 1$ implicit stages. We denote these methods by $GL(2s, s)$ for $s = 1, 2, 3, 4$. We also consider the second order implicit differencing technique proposed for stiff problems in [12] (denoted by KI2). Finally, we consider a commonly used direct Nyström scheme for second order problems: the fourth order A -stable singly diagonally implicit Runge–Kutta–Nyström (SDIRKN4) method with three implicit stages, given in [19].

We compare the above methods with the second and fourth order SBP-SAT schemes considered in section 7.1 for the wave equation in one space dimension. As a first measure of efficiency we simply count the total number of implicit time levels at which the solution is computed. As we can see in Figure 4, the SBP-SAT schemes are slightly more efficient when measured in this way. This comparison, however, does not take into account the added challenge of solving the larger equation system of the global method (this challenge is reduced in the multistage version of SBP-SAT).

For the KI2 and SDIRKN4 methods, only one separate equation system is solved for each implicit time level, leading to small individual systems. In order for the SBP-SAT technique to compete in efficiency on large problems in several dimensions, a suitable iterative technique would be required. To develop such a technique is a nontrivial task due to the highly nonsymmetric and indefinite spectrums of the SBP-SAT discretizations. Both the first and second order forms are quite challenging for standard preconditioning techniques. For this reason, a more detailed investigation taking these differences and related experience into account is beyond the scope of this work. Provided that the challenges mentioned above could be resolved, however, we note that both the global and the multistage SBP-SAT discretizations are well suited for the application of multigrid in space and time.

To illustrate the need for an iterative solution strategy, we show in Figure 5 a measurement of the efficiency in terms of CPU time using the standard direct solver based on LU factorization in MATLAB (the “\” command) and using the multistage version of the SBP-SAT methods. As can be seen, methods employing a single implicit stage are more efficient when measured in this way.

7.3. Nonreflecting boundary conditions. We now consider the case with Robin boundary conditions given by $\beta^2 = 1$ and $a = 1/\beta = 1$ in (16), corresponding to the first order nonreflecting boundary condition of Engquist and Majda [8]. Note that in one space dimension, these conditions are exact. A second order accurate

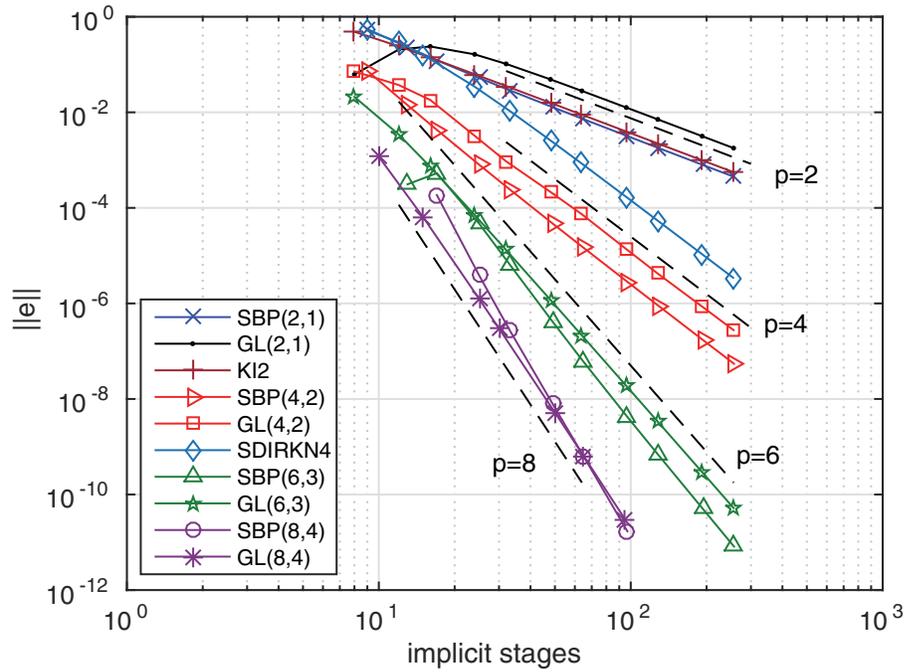


FIG. 2. Convergence of SBP-SAT schemes for the scalar wave equation at $t = 1$.

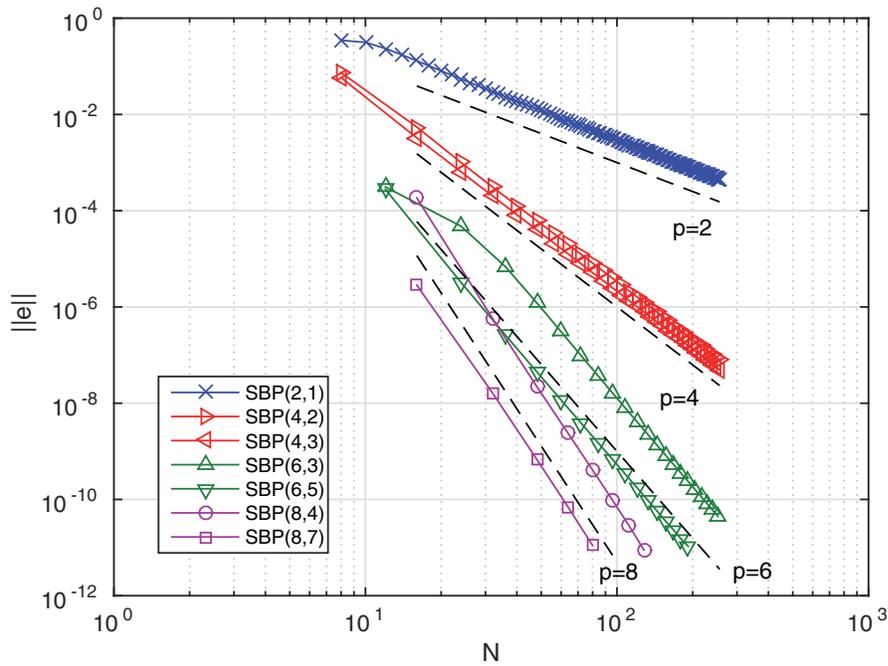


FIG. 3. Convergence of SBP-SAT schemes for the scalar wave equation at $t = 1$ in a multistage version.

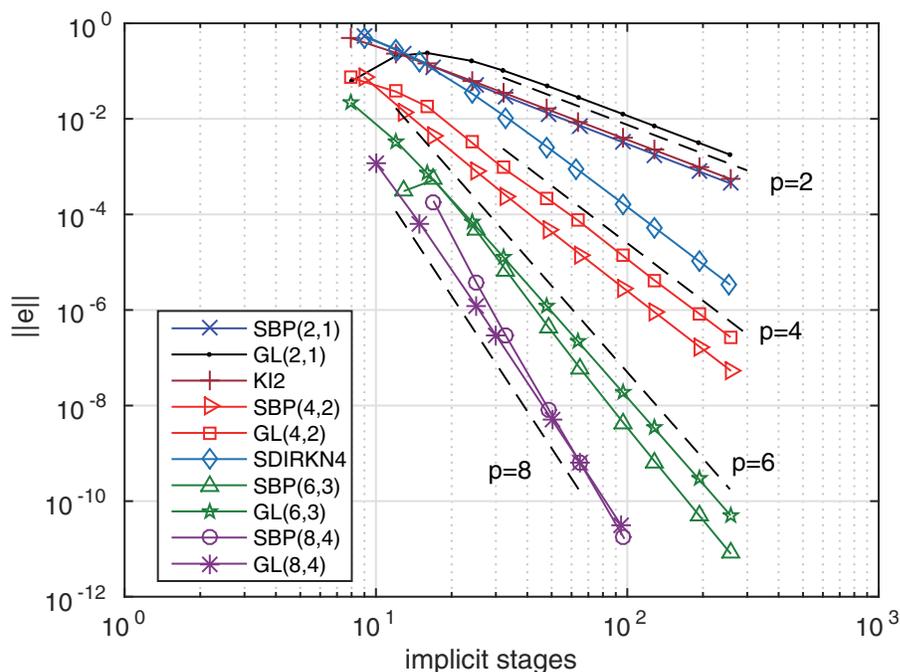


FIG. 4. Efficiency of a collection of unconditionally stable methods for the scalar wave equation as a function of implicit stages. The error is measured at $t = 1$.

explicit difference scheme was proposed for this problem in [8], and we compare this to the new SBP-SAT schemes. We use $\text{SBP}(2s, s)$ in time and $\text{SBP}(2s, 2s - 1)$ in space, thus expecting final solutions accurate to order $2s$. As initial solution we use a Gaussian pulse given by $u = e^{-(12(x-\frac{1}{2}))^2}$ and measure the error at $t = 1$ in the maximum norm. Since the waves originating from the initial solution have left the domain at this point, the exact solution is zero everywhere to machine precision. As we can see in Figure 6, the second order SBP-SAT solution is slightly less accurate than the explicit solution EM2 proposed in [8], but all SBP-SAT solutions converge with the expected order.

As a final illustration we consider the wave equation in two dimensions with first order nonreflecting boundary conditions:

$$\begin{aligned}
 u_{tt} &= u_{xx} + u_{yy}, \\
 u(x, 0) &= f(x), \\
 u_t(x, 0) &= g(x), \\
 u_t(0, y, t) - u_x(0, y, t) &= 0, \\
 u_t(1, y, t) + u_x(1, y, t) &= 0, \\
 u_t(x, 0, t) - u_y(x, 0, t) &= 0, \\
 u_t(x, 1, t) + u_y(x, 1, t) &= 0.
 \end{aligned}
 \tag{42}$$

The spatial and temporal discretizations are carried out in a completely analogous way to the one-dimensional case in section 4 and are not reiterated here. A fourth order accurate solution on a fine grid is obtained by using $\text{SBP}(4, 3)$ in both space

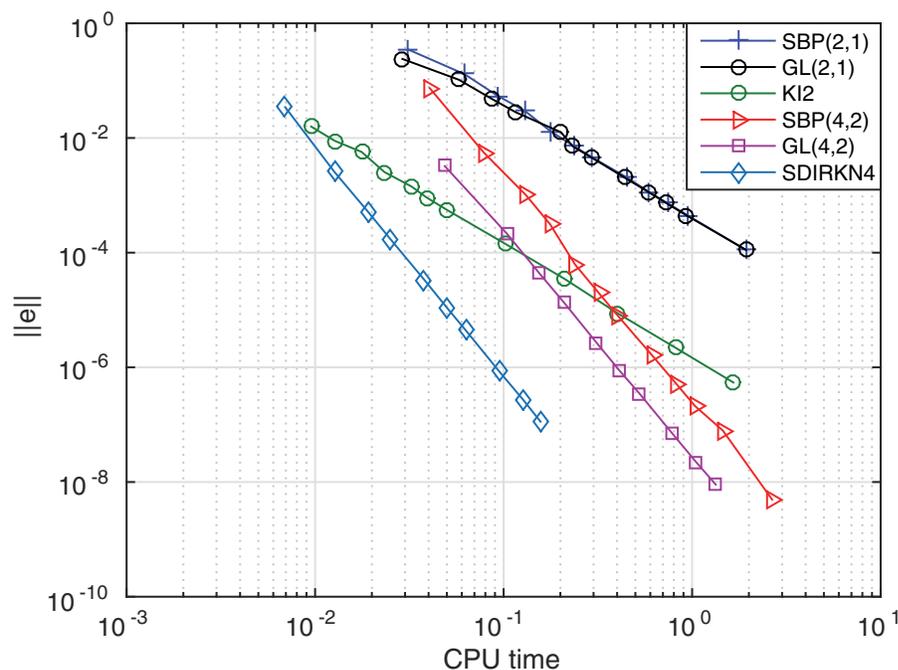


FIG. 5. Efficiency in terms of CPU time of a collection of unconditionally stable methods for the scalar wave equation, using a direct solver. The error is measured at $t = 1$.

and time with $h_x = h_y = h_t = 1/96$. The time integration is divided into 12 separate steps per time unit using the multistage technique. The initial solution in the form of a Gaussian pulse as well as the solution at a few different times are shown in Figure 7. The reflections that can be seen are due to the fact that the boundary conditions used are only approximately nonreflecting for waves approaching the boundaries at an angle.

8. Conclusions. We have demonstrated that high order accurate SBP operators can be used to discretize second order time derivatives in a way that leads to optimal fully discrete energy estimates. The initial conditions are imposed with a modified SAT penalty technique derived from the first order form of the system, together with wide stencil operators in time.

The new method is unconditionally stable, and the implementation can be both fully global in time or in the form of an implicit multiblock/stage time marching scheme. The new methodology also enables the use of mixed boundary conditions in both space and time. This means that nonreflecting boundary conditions, which typically contain time derivatives, can easily be implemented in a provably stable way, using the energy method instead of the more limited normal mode analysis.

We also discuss the possibility of using compact stencil operators in time, but we conclude that they can probably not be incorporated into the technique presented in this paper. The compact operators in compatible form, previously used for spatial approximation, does prove to be a useful framework also for studying temporal operators. Unfortunately, we find that stability cannot be obtained for the second order initial value problem.

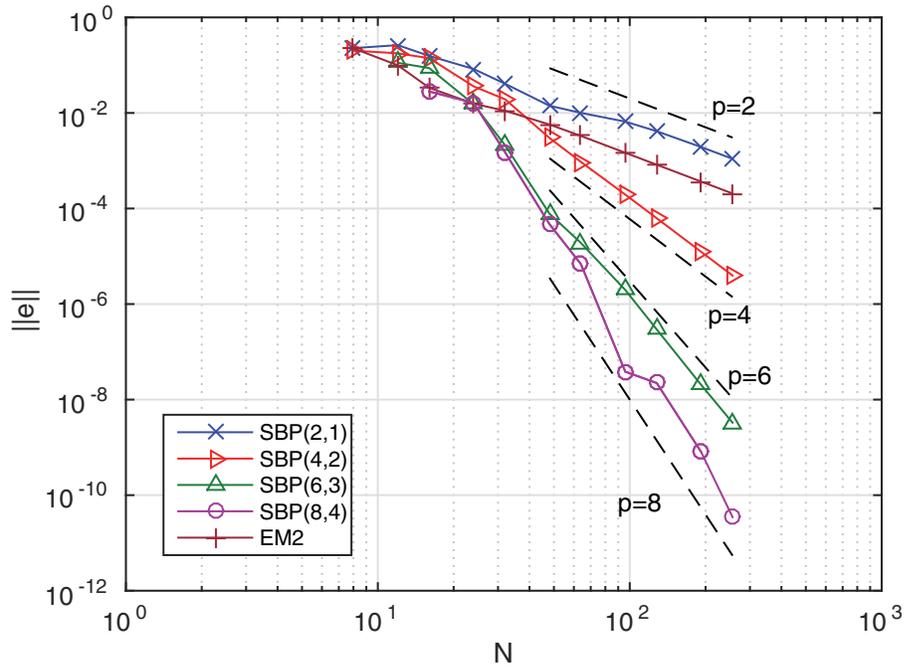


FIG. 6. Convergence for the scalar wave equation with nonreflecting boundary conditions, measured in maximum norm at $t = 1$.

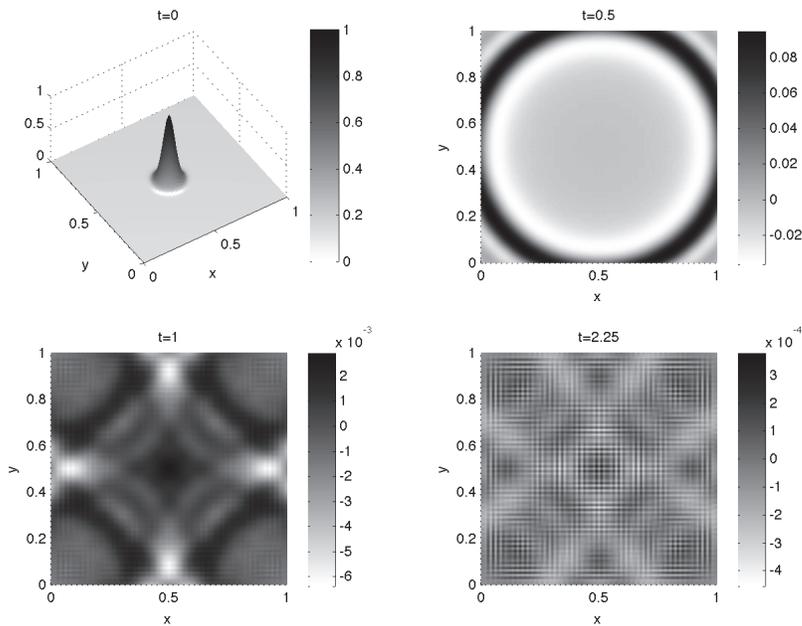


FIG. 7. Solution to the two-dimensional wave equations at different time levels, using SBP(4,3) with grid spacings $h_x = h_y = h_t = 1/96$.

We demonstrate the technique for scalar second order initial value problems as well as for the one- and two-dimensional wave equations with general boundary conditions. The different matrix properties obtained by using both a first and a second order formulation in time is discussed. The numerical results illustrate the stability, accuracy, and efficiency of the new method.

Appendix A. Proof of Lemma 12.

LEMMA 13. *Let A and B be two infinite matrices both consisting of a constant finite length interior stencil centered around the main diagonal. Then A and B commute, i.e., $AB = BA$.*

Proof. Assume that A and B both have $2p + 1$ nonzero elements centered around the main diagonal:

$$A = \begin{pmatrix} \ddots & & & & & & & & \\ & a_{-p} & \dots & a_{-1} & a_0 & a_1 & \dots & a_p & \\ & & \ddots & & & & \ddots & & \\ & & & & & & & & \ddots \\ & & & & & & & & & \ddots \end{pmatrix},$$

$$B = \begin{pmatrix} \ddots & & & & & & & & \\ & b_{-p} & \dots & b_{-1} & b_0 & b_1 & \dots & b_p & \\ & & \ddots & & & & \ddots & & \\ & & & & & & & & \ddots \\ & & & & & & & & & \ddots \end{pmatrix}.$$

Now let $C = AB$, and let $D = BA$. Then the elements in C can be written as

$$c_{-j} = \sum_{q=0}^{2p-j} a_{-p+q} b_{p-j-q}, \quad j = 0, \dots, 2p,$$

$$c_j = \sum_{q=0}^{2p-j} a_{-p+j+q} b_{p-q}, \quad j = 0, \dots, 2p.$$

Similarly, the elements in D can be written as

$$d_{-j} = \sum_{q=0}^{2p-j} b_{-p+q} a_{p-j-q}, \quad j = 0, \dots, p,$$

$$d_j = \sum_{q=0}^{2p-j} b_{-p+j+q} a_{p-q}, \quad j = 0, \dots, p.$$

Now, if we change summation index to $\tilde{q} = 2p - q - j$, then we can rewrite the elements in D as

$$d_{-j} = \sum_{\tilde{q}=0}^{2p-j} b_{p-j-\tilde{q}} a_{-p+\tilde{q}}, \quad j = 0, \dots, p,$$

$$d_j = \sum_{\tilde{q}=0}^{2p-j} b_{-p+\tilde{q}} a_{p-j-\tilde{q}}, \quad j = 0, \dots, p.$$

We see that these are identical to the elements in C . Thus we have $C = D$, i.e., $AB = BA$. \square

Appendix B. The full compact formulation. We now return to the scalar constant coefficient problem (7). A compact formulation is obtained by adding a correction term to the modified discrete second derivative (12), corresponding to the compatible definition (41):

$$(43) \quad \tilde{u}_{tt} = D_1 \tilde{u}_t - P^{-1} R \tilde{u},$$

where $\tilde{u}_t = D_1 \tilde{u} - P^{-1} \tau_0 (u_0 - f) \tilde{e}_0$ as before. As a minimum accuracy requirement, we assume that first order polynomials are differentiated exactly by (43):

$$(44) \quad \begin{aligned} D_1 \vec{1} &= 0, & D_1 \vec{t} &= \vec{1}, \\ R \vec{1} &= 0, & R \vec{t} &= 0. \end{aligned}$$

In (44) we have used $\vec{t} = (0, \Delta x, \dots, N \Delta x, 1)^T$ and $\vec{1} = (1, 1, \dots, 1, 1)^T$.

In order to produce an energy estimate, we again multiply the discrete equation (11) from the left with $\tilde{u}_t^T P$:

$$\begin{aligned} \tilde{u}_{tN}^2 + \beta^2 u_N^2 &= h^2 + \beta^2 f^2 - (\tilde{u}_{t0} - g)^2 - \beta^2 (u_0 - f)^2 \\ &\quad + \tilde{u}^T (D_1^T R + R^T D_1) \tilde{u} + \tau_0 (u_0 - f) \tilde{e}_0^T R \tilde{u}. \end{aligned}$$

Thus, in order to obtain an estimate of the same type as (13) (with possible extra damping from the matrix $D_1^T R + R^T D_1$ and avoiding indefinite terms), the following two conditions must be satisfied:

$$(45) \quad D_1^T R + R^T D_1 \leq 0,$$

$$(46) \quad \tilde{e}_0^T R = 0.$$

A special case where the matrix $D_1^T R + R^T D_1$ in (45) is exactly zero is given by the following operator with a second order compact interior stencil and zeroth order at the boundary:

$$(47) \quad D_2 = \frac{1}{\Delta t^2} \begin{pmatrix} 0 & 0 & 0 & & & \\ 1 & -2 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & & 1 & -2 & 1 \\ & & & 0 & 0 & 0 \end{pmatrix}.$$

Note that (46) above requires the first row of the correction matrix R to be zero. In Lemma 15 below we will also derive an additional condition that is necessary for (45) to hold. To do this we first need the following lemma.

LEMMA 14. *Let A be an $(N + 1)$ by $(N + 1)$ symmetric matrix, and let \vec{x} be a vector such that $\vec{x}^T A \vec{x} = 0$. Then A is indefinite if $A \vec{x} \neq 0$.*

Proof. Note that for $\vec{x} = 0$, the result is trivial. Now, consider for simplicity the case where x_N is nonzero (completely analogous proofs can be formulated assuming any other element to be nonzero). We begin by defining a transformation matrix X as

$$X = (\vec{e}_0, \vec{e}_1, \dots, \vec{e}_{N-1}, \vec{x}) = \begin{pmatrix} 1 & 0 & \dots & 0 & x_0 \\ & 1 & & & x_1 \\ & & \ddots & & \vdots \\ & & & 1 & x_{N-1} \\ & & & & x_N \end{pmatrix}.$$

This leads to the transformation

$$X^T A X = \begin{pmatrix} a_{00} & \dots & a_{0,N-1} & \vec{a}_0^T \vec{x} \\ \vdots & \ddots & & \vdots \\ a_{N-1,0} & & a_{N-1,N-1} & \vec{a}_{N-1}^T \vec{x} \\ \vec{x}^T \vec{a}_0 & \dots & \vec{x}^T \vec{a}_{N-1} & 0 \end{pmatrix},$$

where \vec{a}_j denotes the j th column of A for $j = 0, 1, \dots, N$. Now, since X is nonsingular, A is indefinite if and only if $X^T A X$ is indefinite. Moreover, due to the zero on the last diagonal element, $X^T A X$ must be indefinite unless all elements on the last row and column are zero, i.e., unless $\vec{a}_0^T \vec{x} = \dots = \vec{a}_{N-1}^T \vec{x} = 0$. If this holds, then also $\vec{a}_N^T \vec{x}$ must be zero, since

$$0 = \vec{x}^T A \vec{x} = x_0 \vec{a}_0^T \vec{x} + \dots + x_{N-1} \vec{a}_{N-1}^T \vec{x} + x_N \vec{a}_N^T \vec{x} = x_N \vec{a}_N^T \vec{x}.$$

Thus, A is indefinite unless $\vec{a}_0^T \vec{x} = \dots = \vec{a}_N^T \vec{x} = 0$, i.e., unless $A\vec{x} = 0$. \square

We are now ready to state an additional necessary condition for (45) to be true.

LEMMA 15. *The symmetric matrix $D_1^T R + R^T D_1$ is indefinite unless the following condition holds:*

$$(48) \quad \vec{1}^T P D_2 = (\vec{e}_N - \vec{e}_0)^T D_1,$$

where D_2 is defined in (41).

Proof. We first show that the quadratic form $\vec{t}^T (D_1^T R + R^T D_1) \vec{t}$ is zero. Indeed, using the accuracy conditions (44), we find that

$$\vec{t}^T (D_1^T R + R^T D_1) \vec{t} = 2(D_1 \vec{t})^T (R \vec{t}) = 0.$$

Now assume that $D_1^T R + R^T D_1$ is not indefinite. Then it follows from Lemma 14 that $(D_1^T R + R^T D_1) \vec{t} = 0$, which leads to, again using (44),

$$\begin{aligned} 0 &= (D_1^T R + R^T D_1) \vec{t} = D_1^T (R \vec{t}) + R^T (D_1 \vec{t}) = R^T \vec{1} \\ &\Rightarrow \vec{1}^T R = 0. \end{aligned}$$

Multiplying D_2 from the left with $\vec{1}^T P$ finally gives

$$\begin{aligned} \vec{1}^T P D_2 &= \vec{1}^T Q D_1 - \vec{1}^T R \\ &= \vec{1}^T (B - Q^T) D_1 \\ &= (\vec{e}_N - \vec{e}_0)^T D_1 - (D_1 \vec{1})^T P D_1 \\ &= (\vec{e}_N - \vec{e}_0)^T D_1, \end{aligned}$$

which concludes the proof. \square

We stop here to summarize the results obtained in this section. In order to produce an energy estimate of the same type as (13) (with possible extra damping), the compact operator D_2 given by (41) must satisfy the two conditions (45) and (46). Moreover, we derive in Lemma 15 that (48) is a necessary condition for (46) to hold. We argue that these conditions are not possible to satisfy for compact finite difference interior stencils, and we will motivate this by studying the second order accurate case in more detail.

B.1. Example: The second order accurate case. Inspired by the only single example (47) that we found where condition (45) was satisfied, we will investigate the second order case in detail. From this point on, we assume that a second order accurate compact stencil is employed in the interior of the operator D_2 . If stability cannot be achieved in this special case, it is highly unlikely that higher order accurate operators would perform better.

The standard second order first derivative operator on SBP form is

$$(49) \quad D_1 = \frac{1}{\Delta t} \begin{pmatrix} -1 & 1 & & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & & & \end{pmatrix},$$

and $P = \Delta t \text{Diag}(\frac{1}{2}, 1, \dots, 1, \frac{1}{2})$. This gives the following wide stencil second derivative operator:

$$D_1^2 = \frac{1}{\Delta t^2} \begin{pmatrix} \frac{1}{2} & -1 & \frac{1}{2} & & & \\ \frac{1}{2} & -\frac{3}{4} & 0 & \frac{1}{2} & & \\ \frac{1}{4} & 0 & -\frac{1}{2} & 0 & \frac{1}{4} & \\ & \ddots & & \ddots & & \ddots \end{pmatrix}.$$

In order to satisfy (46), the first row must be the same in D_2 as in D_1^2 , due to the definition of D_2 in (19). For this reason the ansatz for D_2 will be of the following general form, with a second order compact stencil in the interior and an unknown block of size $r > 2$ in the top left corner:

$$(50) \quad D_2 = \frac{1}{\Delta t^2} \begin{pmatrix} \frac{1}{2} & -1 & \frac{1}{2} & & & & \\ \hat{d}_{1,0} & \dots & & \hat{d}_{1,r-1} & & & \\ \vdots & \ddots & & \vdots & & & \\ \hat{d}_{r,0} \dots & & & \hat{d}_{r,r-1} & -2 & 1 & \\ & & & & 1 & -2 & 1 \\ & & & & & \ddots & \ddots & \ddots \end{pmatrix}.$$

To simplify the analysis, we introduce some auxiliary variables. First, the unknown coefficients determining the nonzero pattern in D_2 are collected into a matrix \hat{D}_2 , given by

$$\hat{D}_2 = \begin{pmatrix} \hat{d}_{1,0} & \cdots & \hat{d}_{1,r-1} \\ \vdots & \ddots & \vdots \\ \hat{d}_{r,0} & \cdots & \hat{d}_{r,r-1} \end{pmatrix}.$$

We will also need the first two monomials of the same dimension as \hat{D}_2 :

$$\hat{\mathbf{1}} = (1, 1, \dots, 1)^T, \quad \hat{\mathbf{t}} = (0, 1, 2, \dots, r-1)^T.$$

Using these definitions, the necessary condition (48) along with the accuracy conditions in (44) can now be rewritten into the following three sets of conditions:

$$(51) \quad \hat{\mathbf{1}}^T \hat{D}_2 = \left(\frac{3}{4}, -\frac{1}{2}, -\frac{1}{4}, 0, \dots, 0 \right),$$

$$(52) \quad \hat{D}_2 \hat{\mathbf{1}} = (0, \dots, 0, -1, 1)^T,$$

$$(53) \quad \hat{D}_2 \hat{\mathbf{t}} = (0, \dots, 0, -r, -1+r)^T.$$

Thus we have $3r$ equations for r^2 unknown coefficients in \hat{D}_2 . The three sets of equations above, although consistent, do, however, include linear dependencies. Indeed, if we multiply (52) with $\hat{\mathbf{1}}^T$ from the left, and (51) with $\hat{\mathbf{1}}$ from the right, we obtain one and the same condition:

$$\hat{\mathbf{1}}^T \hat{D}_2 \hat{\mathbf{1}} = 0.$$

Thus we can remove any row in (52) without changing the rank of the full system (51)–(52). Similarly, multiplying (53) with $\hat{\mathbf{1}}^T$ from the left, and (51) with $\hat{\mathbf{t}}$ from the right, we again obtain an identical condition, namely

$$\hat{\mathbf{1}}^T \hat{D}_2 \hat{\mathbf{t}} = -1,$$

and thus we can also remove one arbitrary equation in (53) from the system without losing rank.

The total number of linearly independent equations remaining in (51)–(52) is now $3r - 2$, so the number of free parameters left is $r^2 - 3r + 2$. For instance, if we choose $r = 3$, then \hat{D}_2 can be written using two free parameters as

$$\begin{pmatrix} -\frac{1}{4} & \frac{1}{2} & -\frac{1}{4} \\ 2 & -3 & 0 \\ -1 & 2 & 0 \end{pmatrix} + t_1 \begin{pmatrix} -1 & 2 & -1 \\ 0 & 0 & 0 \\ 1 & -2 & 1 \end{pmatrix} + t_2 \begin{pmatrix} -1 & 2 & -1 \\ 1 & -2 & 1 \\ 0 & 0 & 0 \end{pmatrix}.$$

Using this form of \hat{D}_2 , we have examined numerically whether the upper right corner of $D_1^T R + R^T D_1$ can be negative semidefinite or not. We did this on the parameter domain $-100 \leq t_1, t_2 \leq 100$ with uniform spacing 0.01. The minimum eigenvalue was found to be less than -0.8 for all these parameter values. In fact, the upper left corner of $D_1^T R + R^T D_1$ was indefinite in all cases except one, namely $t_1 = 1$, $t_2 = -2$, in which case the result was *positive* semidefinite.

For $r > 3$, we have used optimization routines in MATLAB to search for negative semidefinite solutions for the cases $r = 4$ and $r = 5$, but without success. We thus find it reasonable to infer that there are no solutions for which $D_1^T R + R^T D_1 \leq 0$. We summarize by stating this conjecture formally.

Conjecture 1. Let D_1 be the second order accurate first derivative operator (49), and let D_2 be a compact second derivative operator defined by (50), under the accuracy constraint given by (44). Then (45) cannot hold together with (46). Thus we cannot obtain an energy estimate on the form (13), even with additional damping.

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