



Summation by parts operators for finite difference approximations of second derivatives

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Abstract

Finite difference operators approximating second derivatives and satisfying a summation by parts rule have been derived for the fourth, sixth and eighth order case by using the symbolic mathematics software Maple. The operators are based on the same norms as the corresponding approximations of the first derivative, which makes the construction of stable approximations to general parabolic problems straightforward. The error analysis shows that the second derivative approximation can be closed at the boundaries with an approximation two orders less accurate than the internal scheme, and still preserve the internal accuracy.

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1. Introduction

High order accurate discretizations of the inviscid flux terms are often required in computational fluid dynamics to efficiently capture the significant flow features, especially for transient problems [5,7,10,13,15,16,20,23,24]. For applications that require the solution to the Navier–Stokes equations, e.g. for separated or turbulent flows, it is essential to approximate the viscous fluxes accurately, too [25]. However, the second derivative terms have received little attention, especially concerning the stability issues for high order approximations [1].

A desirable numerical method has the three main attributes *high order of accuracy*, *simplicity*, and *stability*. Simplicity and high order of accuracy yield efficiency. Stability ensures that the numerical method is well-behaved and that knowledge about the numerical errors are known. One way to obtain a simple, desirable numerical method is to approximate the derivatives of the initial boundary value problem with high order

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accurate, central finite difference operators that satisfy a summation by parts (SBP) formula, and then use the Simultaneous Approximation Term (SAT) method [3], for the implementation of the boundary conditions.

High order accurate SBP operators for the first derivative has previously been developed [11,12] and refined [21]. To construct highly accurate and stable approximations of mixed hyperbolic–parabolic problems, high order accurate SBP operators for the *second* derivative are required, too. For stability reasons, the second derivative approximation must be based on the same norm as the SBP operators approximating the first derivative. SBP operators for the second derivative, based on full norms, have been constructed for the fourth and the sixth order case [4]. However, these operators did not have the optimal SBP property (see Section 2.2). In this paper, we construct SBP operators for the fourth, sixth and eighth order case based on both the full norms and the diagonal norms. In the full norm case, two types of operators for each order of accuracy have been constructed. The first type are closed at the boundary with stencils one order less accurate than the internal scheme, while the second type are closed at the boundary with stencils two orders less accurate.

In Section 2, we discuss the SBP property for both the first and the second derivative and show the construction procedure for the second derivative SBP operator. In Section 3, we analyze the accuracy requirements. In Section 4, we present computations and additional analysis. In Section 5, we draw conclusions. In Appendix A, we briefly discuss second derivative operators and the wave equation. In Appendix B, we consider accuracy requirements for an incompletely parabolic system. In Appendixes C and D, we present the diagonal norm operators and the corresponding full norm operators.

2. Construction of the second derivative

To describe the SBP property in detail, we need the following definitions. Let the inner product for real-valued functions $u, v \in L^2[a, b]$ be defined by $(u, v) = \int_a^b uv \, dx$ and the corresponding norm $\|u\|^2 = (u, u)$. The domain ($a \leq x \leq b$) is discretized using N equidistant grid points,

$$x_j = a + (j - 1)h, \quad j = 1, 2, \dots, N, \quad h = \frac{b - a}{N - 1}.$$

The numerical approximation at grid point x_j is denoted v_j , and the discrete solution vector $v^T = [v_0, v_1, \dots, v_N]$. We define an inner product for discrete real-valued vector-functions $u, v \in \mathbf{R}^n$ by $(u, v)_H = u^T H v$, where $H = H^T > 0$, and a corresponding norm $\|v\|_H^2 = v^T H v$. We will also use the matrices and vectors

$$\begin{aligned} e_0 &= [1, 0, \dots, 0]^T, & E_0 &= \text{diag}([1, 0, \dots, 0]), \\ e_N &= [0, \dots, 0, 1]^T, & E_N &= \text{diag}([0, \dots, 0, 1]). \end{aligned} \tag{1}$$

2.1. The first derivative

An SBP operator mimic the behavior of the corresponding continuous operator with respect to the inner product mentioned above. Consider the hyperbolic scalar equation $u_t + u_x = 0$ (excluding the boundary condition). Note that $(u, u_t) + (u_t, u) = (d/dt)\|u\|^2$. Integration by parts leads to

$$\frac{d}{dt}\|u\|^2 = -(u, u_x) - (u_x, u) = -u^2|_a^b, \tag{2}$$

where we introduce the notation $u^2|_a^b \equiv u^2(x = b) - u^2(x = a)$.

Consider the semidiscrete approximation $v_t + D_1 v = 0$ of the equation. A difference operator $D_1 = H^{-1}Q$ is an SBP operator if $Q + Q^T = B$, where

$$B = \text{diag}(-1, 0, \dots, 0, 1), \tag{3}$$

since this leads to

$$\frac{d}{dt} \|v\|_H^2 = -(v, H^{-1}Qv)_H - (H^{-1}Qv, v)_H = -v^T(Q + Q^T)v = v_0^2 - v_N^2. \tag{4}$$

Eq. (4) is a discrete analog to the integration by parts (IBP) formula (2) in the continuous case.

An SBP operator gives a strict stable approximation for a Cauchy problem. Nevertheless, the SBP property alone does not guarantee strict stability for an initial boundary value problem. Such problems require a specific boundary treatment. Imposing the boundary condition explicitly, i.e., combining the difference operator and the boundary operator into a modified operator, usually destroys the SBP property. In general, this makes it impossible to obtain an energy estimate. This common procedure, *the injection method*, may cause exponential growth of the solution [13,22].

The basic idea behind the Simultaneous Approximation Term (SAT) method [3] and the projection method [18,19] is to impose the boundary conditions such that the SBP property is preserved and an energy estimate can be obtained.

As an example of the simple, yet powerful SAT boundary procedure, we consider the hyperbolic scalar equation

$$u_t + u_x = 0, \quad 0 \leq x \leq 1, \quad t \geq 0, \quad u(0, t) = g_0(t). \tag{5}$$

Integration by parts leads to

$$\frac{d}{dt} \|u\|^2 = g_0^2 - u^2(x = 1). \tag{6}$$

The discrete approximation of (5) using the SAT method for the boundary conditions is

$$v_t + H^{-1}Qv = -H^{-1}\tau\{E_0v - e_0g_0(t)\}, \tag{7}$$

where E_0 and e_0 are defined in (1).

The energy method in (7) leads to

$$\frac{d}{dt} \|v\|_H^2 = \frac{\tau^2}{2\tau - 1} g_0^2 - v_N^2 - (2\tau - 1) \left(v_0 - \frac{\tau}{2\tau - 1} g_0 \right)^2.$$

An energy estimate exist for $\tau > 1/2$. The choice $\tau = 1$ yields

$$\frac{d}{dt} \|v\|_H^2 = g_0^2 - v_N^2 - (v_0 - g_0)^2. \tag{8}$$

Eq. (8) is a discrete analog of the integration by parts formula (6) in the continuous case, where the extra term $(v_0 - g_0)^2$ introduce a small additional damping. Artificial dissipation is not included but can be added in a stable way, see Section 2.2.

There is a variety of SBP operators approximating $\partial/\partial x$ to a certain accuracy, constructed with different norms H [11,12,21]. With a diagonal norm, at most p th order accuracy can be achieved at the boundary, where the internal accuracy is of order $2p$. This will result in a $(p + 1)$ th order accurate approximation of the original problem. With a full norm H (the upper and lower part of the norm consist of $2p$ by $2p$ blocks), a $(2p - 1)$ th order accurate boundary closure exist, which result in a $(2p)$ th order accurate approximation of the original problem. This is due to the fact that it is possible to lower the accuracy by one order at a finite number of points and still obtain accuracy of order $2p$ [8].

2.2. The second derivative

For parabolic problems, we need an SBP operator for the second derivative. Consider the heat equation $u_t = u_{xx}$. Integration by parts leads to

$$\frac{d}{dt} \|u\|^2 = (u, u_{xx}) + (u_{xx}, u) = 2uu_x|_a^b - 2\|u_x\|^2. \quad (9)$$

We base the construction of an SBP operator D_2 approximating $\partial^2/\partial x^2$ in Eq. (9). To fully mimic the IBP property, we need $D_2 = H^{-1}(-D_1^T H D_1 + BS)$, where D_1 is a consistent approximation of $\partial/\partial x$, S includes an approximation of the first derivative operator at the boundary, and B is given by (3). The energy method on the semidiscrete approximation $v_t = D_2 v$ leads to the discrete analog to the IBP formula (see (9)) in the continuous case

$$\frac{d}{dt} \|v\|_H^2 = (v, D_2 v)_H + (D_2 v, v)_H = 2v_N(Sv)_N - 2v_0(Sv)_0 - 2\|D_1 v\|_H^2. \quad (10)$$

However, it is not necessary to fully mimic the IBP property to obtain an energy estimate. Consider the difference operator $H^{-1}(-A + BS)$, approximating $\partial^2/\partial x^2$. The energy method leads to

$$\frac{d}{dt} \|v\|_H^2 = 2v_N(Sv)_N - 2v_0(Sv)_0 - v^T(A + A^T)v. \quad (11)$$

To get an energy estimate it suffice that $A + A^T \geq 0$, assuming that the boundary terms are correctly implemented (see Section 3).

To distinguish between the different forms of the second derivative SBP operators we introduce the following two definitions.

Definition 1. A difference operator $H^{-1}(-A + BS)$ approximating $\partial^2/\partial x^2$ is a second derivative SBP operator if $A + A^T \geq 0$, if S includes an approximation of the first derivative operator at the boundary, and B is given by (3).

Definition 2. A difference operator $H^{-1}(-A + BS)$ approximating $\partial^2/\partial x^2$ is a complete second derivative SBP operator if it is an SBP operator and if $A = D_1^T H D_1$, where D_1 is a consistent approximation of $\partial/\partial x$.

In Appendix A we briefly consider the wave equation, which leads to yet another definition.

Remark. The SBP operators for the second derivative introduced in [4] does not have the optimal SBP property, since $A + A^T \not\geq 0$.

Our goal is, for a mixed hyperbolic–parabolic problems, to construct a difference operator that results in an energy estimate. Then, the SBP operator approximating $\partial^2/\partial x^2$ must be constructed using the same norm (H) as the SBP operator approximating $\partial/\partial x$. To preserve global accuracy, the approximation of the second derivative and the boundary derivative (Sv) must also be accurate enough (discussed further in Section 3).

There are essentially two options for how to construct the SBP operator for the second derivative. The first option is to construct a minimal width operator, which is the main consideration in this paper. The second option is to use the first derivative operator $D_1 = H^{-1}Q$ twice, which we discuss in some detail below.

Using the first derivative twice leads to $H^{-1}(-D_1^T H D_1 + B D_1)$, i.e., a complete second derivative SBP operator (see Definition 2). For the full norm, this approach results in a boundary closure of order $2p - 2$ and a boundary derivative operator BS of order $2p - 1$, where $2p$ is the internal order of accuracy. For the diagonal norm, we obtain a boundary closure of order $p - 1$ and a boundary derivative operator BS of p th order.

Remark. To handle variable diffusion terms such as $(au_x)_x$, where a is non-constant, we could use the first derivative approximation twice, i.e., form $D_1 A D_1$, since this leads to a discrete analog to the IBP formula.

Compared to the minimal width operator, using the first derivative twice has some drawbacks. Firstly, the internal width of the scheme increases from $2p + 1$ to $4p + 1$. Secondly, the internal error constant is $2p + 2$ times larger. Finally, since the π -mode (the highest frequency that can exist on the grid) is not modified (not “seen”) with a centered, odd-order difference operator, like $H^{-1}Q$, it also holds for the product $(H^{-1}Q)^2$. This causes problems, since the π -mode is primarily responsible for the spurious oscillations (causing the aliasing error) in the solution. One solution is to combine the first derivative operator $H^{-1}Q$ with a special SBP-preserving artificial dissipation operator $DI = H^{-1}R$ (see [15]) to construct an upwind operator $D_+ = H^{-1}(Q + R)$ and a downwind operator $D_- = H^{-1}(Q - R)$, where $R = R^T \geq 0$. By using these operators, we can construct an upwind-based SBP operator for the second derivative

$$D_2^{(u)} = \frac{1}{2}(D_+D_- + D_-D_+) = H^{-1}(-D_1^T H D_1 + B D_1) - H^{-1}(D I^T H D I),$$

where the extra term $-H^{-1}(D I^T H D I)$ introduce damping. Due to the construction of DI , this operator efficiently “kills” the π -mode without destroying the accuracy of the method. This completes the discussion on using the first derivative twice. We now continue with the minimal width operators.

2.3. The construction

This section briefly describes the construction of the second derivative SBP operators (see Definition 1). Here, the accuracy and symmetry requirements on the second derivative operator are assumed given (motivated later). The form of the operator is given by $D_2 = H^{-1}(-A + BS)$, where $A + A^T \geq 0$, S is the boundary derivative operator, and H is the norm given from the corresponding first derivative SBP operator ($D_1 = H^{-1}Q$). The requirement for minimal width (the same width and internal order of accuracy as the corresponding first derivative approximation) implies a given interior scheme. It remains to find the boundary modification such that:

- D_2 is accurate enough at the boundaries,
- S is accurate enough, and
- $A + A^T \geq 0$.

The accuracy at the boundary depends on the type of norm used. Let $2p$ denote the internal accuracy (or design order) of the scheme. For the full norm, the first derivative approximation have a boundary closure of order $2p - 1$. However, as will be shown in Section 3, it is enough to close the boundaries of the second derivative approximation with stencils of order $2p - 2$ and use a boundary derivative approximation of order $2p - 1$, to preserve the design order of accuracy. For the diagonal norm, the first derivative SBP operator is only p th order accurate at the first $2p$ boundary points, leading to less restrictive accuracy requirements of the corresponding second derivative approximation. The structure of A is shown in Fig. 1.

A =

M	C	0
C^T	D	C^T
0	C[~]	M[~]

Fig. 1. The structure of A in the second derivative SBP operator.

The bar is here defined as a permutation of both rows and columns, i.e

$$P = \begin{bmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \end{bmatrix} \Rightarrow \bar{P} = \begin{bmatrix} P_{23} & P_{22} & P_{21} \\ P_{13} & P_{12} & P_{11} \end{bmatrix}.$$

Here (see Fig. 1) \mathbf{M} is a $2p \times 2p$ matrix to be computed and

$$\mathbf{D} = \begin{bmatrix} d_0 & \cdots & d_p & & & \\ \vdots & \ddots & & \ddots & & \\ d_p & \cdots & d_0 & \cdots & d_p & \\ & \ddots & & \ddots & & \\ & & d_p & \cdots & d_0 & \cdots & d_p \\ & & & \ddots & & \ddots & \\ & & & & d_p & \cdots & d_0 \end{bmatrix} \quad \mathbf{C} = \begin{bmatrix} C_0 & 0 \cdots \\ C_s & 0 \cdots \end{bmatrix} \quad (12)$$

$$C_s = \begin{bmatrix} d_p & & & & \\ d_{p-1} & d_p & & & \\ \vdots & & \ddots & & \\ d_1 & \cdots & \cdots & d_p \end{bmatrix},$$

where C_0 is a $p \times p$ zero matrix. The middle part, $h^{-1}(\mathbf{C}^T \mathbf{D} \bar{\mathbf{C}}^T)$, represents the interior scheme of the second derivative SBP operator, i.e., the minimal width central scheme of order $2p$. The boundary derivative operator has the form

$$S = \begin{bmatrix} -s_1 & \cdots & -s_r & 0 \cdots \\ & 1 & & \\ & & \ddots & \\ & & & 1 \\ \cdots & 0 & s_r & \cdots & s_1 \end{bmatrix}.$$

The order restriction on S leads to a linear relation between the unknowns $s_i, i = 1 \dots r$. Note that a p th order accurate first derivative approximation requires at least $p + 1$ unknowns. The $2p$ first and last rows in $D_2 = H^{-1}(-A + BS)$ represent the boundary part of the second derivative operator, with the undetermined coefficients coming from M and S . The order requirement on D_2 leads to a linear equation system. If a solution exist, the rest of the undetermined coefficients are tuned such that $A + A^T \geq 0$.

To construct the diagonal norms-based second derivative SBP operators (see Definition 1), we make the following assumptions. (1) Operators with p th order accuracy at the boundaries (the same accuracy as the corresponding first derivative SBP operators) exist, (2) $A = A^T$, since a symmetric A is desirable (see Fig. 1 and Appendix A). Given these assumptions, we used the symbolic mathematics software Maple to construct symmetric SBP operators (see Definition A.2) for the second, fourth, sixth and eighth order diagonal norm (see Appendix C).

Due to the more demanding accuracy conditions, constructing second derivative SBP operators for the full norm is more complicated. We assume that (1) there exist second derivative SBP operators of order $2p - 2$ at the boundaries, and (2) S is $(2p - 1)$ th order accurate. Under the assumption $A = A^T$, no solutions could be found, even if we increased the size of M (see Fig. 1). But with a non-symmetric A , solutions exist for the fourth, sixth and eighth order full norm (see Appendix D).

To study the accuracy requirements, we also constructed full norm SBP operators one order more accurate than the previous, i.e., with boundary closures of order $2p - 1$ and $(2p)$ th order accurate boundary derivatives [14].

3. Accuracy requirements

In this section the accuracy requirements of the difference approximations and the boundary approximations are analyzed by considering a parabolic problem. Consider the advection–diffusion equation

$$\begin{aligned}
 u_t + au_x &= \epsilon u_{xx}, \quad 0 \leq x \leq 1, \quad t \geq 0, \quad u(x, 0) = f(x), \\
 \alpha u(0, t) + u_x(0, t) &= g_0(t), \quad \beta u(1, t) + u_x(1, t) = g_1(t),
 \end{aligned}
 \tag{13}$$

where $a, \epsilon > 0$. The energy method applied to (13) leads to

$$\begin{aligned}
 \frac{d}{dt} \|u\|^2 &= -(a + 2\epsilon\beta) \left(u(1, t) - \frac{\epsilon}{a + 2\epsilon\beta} g_1(t) \right)^2 + \frac{\epsilon^2}{a + 2\epsilon\beta} g_1(t)^2 \\
 &+ (a + 2\epsilon\alpha) \left(u(0, t) - \frac{\epsilon}{a + 2\epsilon\alpha} g_0(t) \right)^2 - \frac{\epsilon^2}{a + 2\epsilon\alpha} g_0(t)^2 - 2\epsilon \|u_x\|^2.
 \end{aligned}
 \tag{14}$$

An energy estimate exists for

$$a + 2\epsilon\beta > 0, \quad a + 2\epsilon\alpha < 0.
 \tag{15}$$

The discrete approximation of (13) using the SAT method for the boundary conditions leads to

$$\begin{aligned}
 v_t + aH^{-1}Qv &= \epsilon H^{-1}(-A + BS)v - H^{-1}\tau_0\{E_0(\alpha I + S)v - e_0g_0(t)\} \\
 &- H^{-1}\tau_1\{E_N(\beta I + S)v - e_Ng_1(t)\}, \quad v(0) = f,
 \end{aligned}
 \tag{16}$$

where E_0, E_N, e_0 and e_N are defined in (1). The energy method applied to (16) leads to

$$\begin{aligned}
 \frac{d}{dt} \|v\|_H^2 &= -(a + 2\tau_1\beta) \left(v_N - \frac{\tau_1}{a + 2\tau_1\beta} g_1 \right)^2 + \frac{\tau_1^2}{a + 2\tau_1\beta} g_1^2 + (a - 2\tau_0\alpha) \left(v_0 - \frac{\tau_0}{a - 2\tau_0\alpha} g_0 \right)^2 \\
 &- \frac{\tau_0^2}{a - 2\tau_0\alpha} g_0^2 + 2(Sv)_N(\epsilon - \tau_1) - 2(Sv)_0(\epsilon + \tau_0) - 2\epsilon v^T(A + A^T)v.
 \end{aligned}$$

An energy estimate (analog to the continuous case (14)) is obtained if $A + A^T \geq 0$ (see Definition 1) and

$$\tau_0 = -\epsilon, \quad \tau_1 = \epsilon.
 \tag{17}$$

We are interested in an estimate of the error. If we insert the true solution $u(x, t)$ into the numerical scheme (16) and subtract (16) we obtain the error equation

$$e_t = Me + T, \quad e(0) = 0,
 \tag{18}$$

where

$$M = H^{-1}(-aQ + \epsilon(-A + BS) - \tau_0E_0(\alpha + S) - \tau_1E_N(\beta + S)).$$

In (18),

$$T = [\mathcal{O}(h^r), \dots, \mathcal{O}(h^r), \mathcal{O}(h^{2p}), \dots, \mathcal{O}(h^{2p}), \mathcal{O}(h^r), \dots, \mathcal{O}(h^r)]^T
 \tag{19}$$

is the truncation error, with contributions from the approximation of the derivatives and the approximation of the boundary derivatives (Su) in the penalty terms. Note that $r < 2p$. If (15) and (17) hold the semidiscrete approximation (18) will result in an energy estimate, which gives us an error estimate directly by using the energy method in (18). However, due to the boundary error, this will result in the estimate $\|e\| \leq \mathcal{O}(h^r)$, which is not sharp.

To obtain an optimal error estimate, the error is split into two parts $e = e_i + e_b$, where the subscripts (i,b) denotes the inner and the boundary points, respectively. The truncation error is divided correspondingly, i.e., $T = T_i + T_b$, where

$$\begin{aligned} T_i &= [0, \dots, 0, \mathcal{O}(h^{2p}), \dots, \mathcal{O}(h^{2p}), 0, \dots, 0]^T, \\ T_b &= [\mathcal{O}(h^r), \dots, \mathcal{O}(h^r), 0, \dots, 0, \mathcal{O}(h^r), \dots, \mathcal{O}(h^r)]^T. \end{aligned} \quad (20)$$

Lemma 1. *If (15) and (17) hold in (16), (18), then*

$$\|e_i\|_H \leq \mathcal{O}(h^{2p}). \quad (21)$$

Proof. The equation for the inner part of the error is given by (18), where e now denotes e_i and T denotes T_i . The energy method applied to (18) leads directly to

$$\|e_i\|_H \leq \frac{\exp(\frac{\eta t}{2})}{\sqrt{\eta}} (\|T_i\|_H)_{\max(0,t)} = \mathcal{O}(h^{2p}),$$

(where η is an arbitrary positive constant) if (17) and (15) hold. \square

To estimate e_b , we use the Laplace transform technique [9]. Laplace transformation of (18), where only e_b is considered, leads to

$$s\widehat{e}_b - M\widehat{e}_b = T_b. \quad (22)$$

In this case it is natural to multiply (22) by h^2 and introduce $\tilde{s} = sh^2$, $\tilde{T}_b = h^2 T_b$ and $\tilde{M} = Mh^2$.

Remark. For a hyperbolic problem $\tilde{s} = sh$, $\tilde{T}_b = hT_b$ and $\tilde{M} = Mh$, since this means that the coefficients in \tilde{M} are of $\mathcal{O}(1)$. The analysis would otherwise follow the path shown below, see [8].

We now rewrite (22) as

$$P\widehat{e}_b = \tilde{T}_b, \quad (23)$$

where $P = \tilde{s}I - \tilde{M}$ (I is the identity matrix). An SBP operator (approximating either the first or the second derivative), $(2p)$ th order accurate in the interior, has two boundary blocks of size $(2p \times 3p)$, which we denote $P^{(l,r)}$ (where (l,r) denotes the left and the right boundary, respectively). Recall that \tilde{T}_b is zero in the interior. The solution to (23) can be written as

$$(\widehat{e}_b)_j = \sum_{i=1}^{2p} \sigma_i \kappa_i^j, \quad (24)$$

where κ_i , $i = 1, \dots, 2p$ are given by solving the characteristic equation (determined by the internal difference scheme) and the unknowns σ_i are determined by the remaining equations, corresponding to the boundary blocks.

We seek conditions for which σ_i , $i = 1, \dots, 2p$ are bounded and proportional to h^{r+2} , since this leads to $\|e_b\| = \mathcal{O}(h^{2p})$, which means that we can have $r = 2p - 2$, and still obtain accuracy of order $2p$.

We need exactly $2p$ equations to solve for the $2p$ unknowns σ_i . However, each boundary block $P^{(l,r)}$ has $2p$ rows (i.e., $4p$ in total) and the set of equations must be reduced. Let

$$\begin{aligned} \hat{e}_1^{(l)} &\equiv [(\hat{e}_b)_1, \dots, (\hat{e}_b)_p]^T, & \tilde{T}_1^{(l)} &\equiv [(\tilde{T}_b)_1, \dots, (\tilde{T}_b)_p]^T, \\ \hat{e}_2^{(l)} &\equiv [(\hat{e}_b)_{p+1}, \dots, (\hat{e}_b)_{3p}]^T, & \tilde{T}_2^{(l)} &\equiv [(\tilde{T}_b)_{p+1}, \dots, (\tilde{T}_b)_{2p}]^T, \\ \hat{e}_1^{(r)} &\equiv [(\hat{e}_b)_{N-p+1}, \dots, (\hat{e}_b)_N]^T, & \tilde{T}_1^{(r)} &\equiv [(\tilde{T}_b)_{N-p+1}, \dots, (\tilde{T}_b)_N]^T, \\ \hat{e}_2^{(r)} &\equiv [(\hat{e}_b)_{N-3p+1}, \dots, (\hat{e}_b)_{N-p}]^T, & \tilde{T}_2^{(r)} &\equiv [(\tilde{T}_b)_{N-3p+1}, \dots, (\tilde{T}_b)_{N-p}]^T, \end{aligned}$$

and let

$$P^{(l)} = \begin{bmatrix} P_{11}^{(l)} & P_{12}^{(l)} \\ P_{21}^{(l)} & P_{22}^{(l)} \end{bmatrix}, \quad P^{(r)} = \begin{bmatrix} P_{22}^{(r)} & P_{21}^{(r)} \\ P_{12}^{(r)} & P_{11}^{(r)} \end{bmatrix}, \tag{25}$$

where $P_{11}^{(l,r)}, P_{21}^{(l,r)}$ are $p \times p$ -matrices and $P_{12}^{(l,r)}, P_{22}^{(l,r)}$ are $p \times 2p$ -matrices. The $4p$ equations can be written as

$$\begin{aligned} P_{11}^{(l,r)} \hat{e}_1^{(l,r)} + P_{12}^{(l,r)} \hat{e}_2^{(l,r)} &= \tilde{T}_1^{(l,r)}, \\ P_{21}^{(l,r)} \hat{e}_1^{(l,r)} + P_{22}^{(l,r)} \hat{e}_2^{(l,r)} &= \tilde{T}_2^{(l,r)}. \end{aligned} \tag{26}$$

If $P_{21}^{(l,r)}$ is non-singular (notice that $P_{21}^{(l,r)}$ is independent of \tilde{s}), (26) can be reduced to

$$B^{(l,r)} \hat{e}_2^{(l,r)} = \tilde{T}_f^{(l,r)},$$

where

$$B^{(l,r)} = P_{12}^{(l,r)} - P_{11}^{(l,r)} (P_{21}^{(l,r)})^{-1} P_{22}^{(l,r)}, \quad \tilde{T}_f^{(l,r)} = \tilde{T}_1^{(l,r)} - P_{11}^{(l,r)} (P_{21}^{(l,r)})^{-1} \tilde{T}_2^{(l,r)}.$$

This leads to a linear system of equations

$$C(\tilde{s}) \sigma = \tilde{T}_f, \tag{27}$$

where

$$\tilde{T}_f^T = \left[[\tilde{T}_f^{(l)}]^T, [\tilde{T}_f^{(r)}]^T \right]$$

and

$$C(\tilde{s}) = \begin{bmatrix} \sum_{i=1}^{2p} b_{1,i}^{(l)} \kappa_1^{p+i} & \cdots & \sum_{i=1}^{2p} b_{1,i}^{(l)} \kappa_{2p}^{p+i} \\ \vdots & & \vdots \\ \sum_{i=1}^{2p} b_{p,i}^{(l)} \kappa_1^{p+i} & \cdots & \sum_{i=1}^{2p} b_{p,i}^{(l)} \kappa_{2p}^{p+i} \\ \sum_{i=1}^{2p} b_{1,i}^{(r)} \kappa_1^{N-3p+i} & \cdots & \sum_{i=1}^{2p} b_{1,i}^{(r)} \kappa_{2p}^{N-3p+i} \\ \vdots & & \vdots \\ \sum_{i=1}^{2p} b_{p,i}^{(r)} \kappa_1^{N-3p+i} & \cdots & \sum_{i=1}^{2p} b_{p,i}^{(r)} \kappa_{2p}^{N-3p+i} \end{bmatrix}, \quad \sigma = \begin{bmatrix} \sigma_1 \\ \vdots \\ \sigma_{2p} \end{bmatrix}. \tag{28}$$

Remark. For a $(2p)$ th order accurate method it is necessary to modify p equations close to the boundary. The additional p equations required for the SBP operators make the reduction discussed above necessary.

Lemma 2. If $C(\tilde{s})$ in (27) is non-singular for $Re \tilde{s} \geq 0$, $P_{21}^{(l,r)}$ in (26) is non-singular and $r = 2p - 2$, then

$$\|e_b\|_H = \mathcal{O}(h^{2p}). \tag{29}$$

Proof. Multiplying (16) by h^2 implies that the coefficients in $\tilde{M} = Mh^2$ (see (23)) are proportional to $(\gamma_1 + \gamma_2 h)$, where γ_1 and γ_2 are constants of order one. This means that the solution to (27) has terms proportional to $(\gamma_1 + \gamma_2 h)^{-1} h^{r+2}$ if $C(\tilde{s}) \neq 0$. If the grid size h is sufficiently small, $(\gamma_1 + \gamma_2 h)^{-1} \approx 1/\gamma_1 - (\gamma_2/\gamma_1^2)h$. Using Parseval's relation and relation (24) we obtain (29). \square

Remark. Lemma 2 holds also for a hyperbolic problem if we replace $r = 2p - 2$ with $r = 2p - 1$.

We are now ready to tie everything together in the following proposition

Proposition 3.1. Consider the advection–diffusion equation (13) and the corresponding semidiscrete problem (16). The error equation is given by (18), (19). If the estimates (21), (29) hold, then

$$\|e\|_H = \mathcal{O}(h^{2p}). \quad (30)$$

Proof. The triangle inequality leads directly to (30). \square

Proposition 3.1 states that a stable implementation of a parabolic problem satisfying Lemmas 1 and 2 allows us to: (i) use one order less accurate approximations, compared to the internal accuracy, of the physical boundary conditions, (ii) close the first and the second derivative approximations with stencils that are two orders less accurate than the internal scheme, and still maintain the design order of accuracy.

4. Computations and further analysis

4.1. A scalar hyperbolic–parabolic problems

To test the convergence rate of the semidiscrete approximation of advection–diffusion equation (13) we choose an analytic solution to the Cauchy problem

$$u = \sin(w(x - ct))e^{-bx}, \quad c > 0, \quad w = \frac{\sqrt{c^2 - a^2}}{2\epsilon}, \quad b = \frac{c - a}{2\epsilon}, \quad |c| > |a|. \quad (31)$$

To truncate the domain we introduce boundary conditions at $x = 0$ and $x = 1$. The convergence rate is calculated as

$$q = \log_{10} \left(\frac{\|u - v^{h1}\|_h}{\|u - v^{h2}\|_h} \right) / \log_{10} \left(\frac{h_1}{h_2} \right), \quad (32)$$

where u is the analytic solution and v^{h1} the corresponding numerical solution with grid size h_1 . $\|u - v^{h1}\|_h$ is the l_2 –error.

The convergence studies for the fourth and sixth order case are shown in Tables 1 and 2, where the convective terms have been treated with one order less accurate boundary closures, compared to the internal accuracy. Two types of second derivative approximations have been tested for each order of accuracy. The first approximation is closed at the boundaries with stencils two orders less accurate, compared to the internal accuracy. The second type is closed with one order less accurate approximations at the boundaries, compared to the internal accuracy. For each computation we have included the case where the stability conditions (17) are violated by choosing $\tau_0 = -\epsilon/2$, such that the energy estimate no longer holds. In the computations presented in Tables 1–3 we have chosen $a = 1$, $c = 2$, $\epsilon = 0.1$ and $\alpha = 1$, $\beta = 0$ (see (13)). The solutions are advanced in time using the standard fourth order Runge–Kutta method.

The error analysis requires that the numerical approximation results in an energy estimate. If we violate (17) such that an energy estimate no longer exists, one order of accuracy is lost if the second derivative

Table 1
 $\log(l_2\text{-error})$ and convergence rate for the fourth order case, based on the block norm

N	l_2	q	l_2^v	q^p
(a) Second order boundary closure ^a				
40	-4.31		-3.11	
60	-5.06	4.14	-3.67	3.11
100	-5.98	4.09	-4.36	3.08
200	-7.20	4.04	-5.28	3.04
300	-7.91	4.02	-5.82	3.03
(b) Third order boundary closure				
40	-4.24		-3.84	
60	-4.97	4.09	-4.58	4.09
100	-5.89	4.06	-5.48	4.02
200	-7.11	4.04	-6.69	3.98
300	-7.82	4.02	-7.39	3.98

In the computations marked v , (17) is violated by choosing $\tau_0 = -\epsilon/2$.

^aNote the loss of convergence.

Table 2
 $\log(l_2\text{-error})$ and convergence rate for the sixth order case, based on the block norm

N	l_2	q	l_2^v	q^p
(a) Fourth order boundary closure ^a				
40	-5.80		-4.46	
60	-6.84	5.75	-5.32	4.78
80	-7.58	5.86	-5.94	4.87
100	-8.16	5.98	-6.42	4.91
120	-8.66	6.27	-6.81	4.94
(b) Fifth order boundary closure				
40	-5.73		-4.83	
60	-6.75	5.68	-5.87	5.82
80	-7.49	5.79	-6.62	5.92
100	-8.06	5.86	-7.21	5.96
120	-8.54	5.92	-7.68	5.98

In the computations marked v , (17) is violated by choosing $\tau_0 = -\epsilon/2$.

^aNote the loss of convergence.

approximation is closed at the boundaries with two orders less accurate stencils, compared to the internal accuracy. Table 3 shows the results for the fourth order diagonal norm case, where also the approximation of the first derivative has a boundary closure two orders less accurate than the internal scheme.

The numerical study shows (indicated by the analysis in Section 3) that a difference approximation for a parabolic problem retains the design order of accuracy if an energy estimate exists and

- two orders less accurate boundary closures are used, compared to the internal accuracy, for both the first and the second derivative approximations;
- the physical boundary conditions are approximated with one order less accurate approximations, compared to the internal accuracy.

Remark. By using a numerical algorithm we have verified that the conditions in Lemma 2 hold for the semidiscrete approximations of (13), used in the convergence study (Tables 1–3).

One might suspect that the loss of accuracy (shown in Tables 1–3) could have something to do with an instability in the method since the energy estimate is lost. But an eigenvalue analysis shows that the methods

Table 3

$\log(l_2\text{-error})$ and convergence rate for the fourth order case, based on the diagonal norm, with second order boundary closure for both the first and the second derivative approximations

N	l_2	q	l_2^v	q^v
40	-4.25		-2.59	
60	-5.02	4.30	-3.13	3.01
100	-5.98	4.25	-3.81	3.01
200	-7.24	4.17	-4.72	3.01
300	-7.97	4.11	-5.25	3.00

In the computations marked v , (17) is violated by choosing $\tau_0 = -\epsilon/2$. Note the loss of convergence, right-hand side (columns 4 and 5).

are stable and that the discrete spectrum converges to the continuous eigenvalues at the same rate as the l_2 -error in Tables 1–3.

In [4] a similar convergence study was done for the nonlinear Burgers' equation. The results for the fourth order accurate case showed that a boundary closure with stencils of second order accuracy reduced the overall convergence rate to third order. This motivated us to perform similar computations. The results of that study (not presented here) agreed well with our previous computations for the linear advection–diffusion problem, i.e., a boundary closure with stencils of second order accuracy yield an overall convergence rate of fourth order. We also tuned the penalty parameters such that the stability conditions were violated. This again resulted in an overall convergence rate of third order. The loss of accuracy in [4] could possibly be due to an non-optimal choice of penalty parameters.

In Table 4, a convergence study for a hyperbolic problem (5) is presented. The results show, in agreement with [8], that in order to preserve the internal accuracy of the scheme we must close the boundaries with at most one order less accurate stencils.

4.2. An incompletely parabolic system

The results of the previous sections, i.e., the accuracy requirements on the boundary closures for parabolic and hyperbolic problems motivated us to investigate an incompletely parabolic system.

4.2.1. The continuous problem

Consider the incompletely parabolic system

$$u_t + Cu_x = Du_{xx}, \quad (33)$$

Table 4

$\log(l_2\text{-error})$ and convergence rate for a hyperbolic problem

N	l_2	q
(a) Fourth order diagonal norm, second order boundary closure		
40	-2.15	
60	-2.70	3.05
100	-3.38	3.02
200	-4.29	3.01
300	-4.82	3.01
(b) Fourth order full norm, third order boundary closure		
40	-2.77	
60	-3.49	3.99
100	-4.38	3.96
200	-5.58	3.98
300	-6.29	3.98

where

$$u = \begin{bmatrix} u^{(1)} \\ u^{(2)} \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad D = \begin{bmatrix} 0 & 0 \\ 0 & \epsilon \end{bmatrix}, \quad \epsilon > 0.$$

We consider (33) to be a model of the compressible Navier–Stokes equations. The energy method is used to derive suitable boundary conditions. When characteristic boundary conditions are used for incomplete parabolic systems (like the Navier–Stokes equations or Eq. (33)), there are some theoretical problems, see [17]. The matrix C is symmetric with distinct eigenvalues and orthogonal eigenvectors. The diagonal form of C is $R^T A R$ where

$$A = \begin{bmatrix} \sqrt{2} & 0 \\ 0 & -\sqrt{2} \end{bmatrix}, \quad R = \begin{bmatrix} \frac{\sqrt{2}+1}{\sqrt{4+2\sqrt{2}}} & \frac{1}{\sqrt{4+2\sqrt{2}}} \\ -\frac{\sqrt{2}-1}{\sqrt{4-2\sqrt{2}}} & \frac{1}{\sqrt{4-2\sqrt{2}}} \end{bmatrix}. \tag{34}$$

An equation on symmetric characteristic form is obtained by multiplying (33) by the matrix R . The result is

$$v_t + A v_x = \tilde{D} v_{xx}, \tag{35}$$

where $v = R u$ and

$$\tilde{D} = \frac{\epsilon}{2\sqrt{2}} \begin{bmatrix} \sqrt{2}-1 & 1 \\ 1 & \sqrt{2}+1 \end{bmatrix}.$$

Artificial boundaries are introduced at $x = 0, 1$ and the full problem becomes

$$\begin{aligned} v_t + A v_x &= \tilde{D} v_{xx} + F(x, t), & 0 \leq x \leq 1, \quad t \geq 0, \\ L_0 v &= g_0(t), & x = 0, \quad t \geq 0, \\ L_1 v &= g_1(t), & x = 1, \quad t \geq 0, \\ v(x, 0) &= f(x), & 0 \leq x \leq 1, \quad t = 0. \end{aligned} \tag{36}$$

In (36) L_0, L_1 are the boundary operators to be determined. For completeness we have also included a forcing function F . The energy method on (36) leads to

$$\frac{d}{dt} \|v\|^2 = B T_{x=0} - B T_{x=1} + \eta \|v\|^2 + \frac{1}{\eta} \|F\|^2 - 2 \int_0^1 v_x^T \tilde{D} v_x \, dx,$$

where $\eta > 0$ and

$$B T = v^T (A v - 2 \tilde{D} v_x) = [v, \quad v_x] [Q] [v, \quad v_x]^T, \quad Q = \begin{bmatrix} A & -\tilde{D} \\ -\tilde{D} & 0 \end{bmatrix}. \tag{37}$$

To simplify the analysis we consider homogeneous boundary conditions ($g_0 = g_1 = 0$). To obtain a well posed problem, $B T_{x=0} \leq 0$ and $B T_{x=1} \geq 0$ are required. The boundary terms (37) can be written in the following way:

$$B T = \sum_{i=1}^2 \lambda_i^{-1} \{ (\lambda_i v_i - G_i)^2 - G_i^2 \}, \tag{38}$$

where $\lambda_1 = \sqrt{2}, \lambda_2 = -\sqrt{2}$ and $[G_1 \ G_2]^T = \tilde{D} v_x$. The number of boundary conditions at hand are given by the eigenvalues of the matrix Q in (37). It can be shown that Q have two positive, one negative and one zero eigenvalue. This implies that we have to specify two boundary conditions at $x = 0$ and one boundary condition at $x = 1$. A maximally dissipative set of boundary conditions at $x = 0$ are $v_1 \lambda_1 - G_1 = 0, G_2 = 0$ (since $\lambda_1 > 0, \lambda_2 < 0$). At $x = 1$ we are only allowed to specify one boundary condition, and at first it seems impossible to get $B T_{x=1} \geq 0$. However, \tilde{D} is linearly dependent and $G_1 = \alpha G_2$ with $\alpha = \sqrt{2} - 1$. By choosing $v_2 \lambda_2 - G_2 = 0$ as a boundary condition and use the relation $G_2 = G_1 / \alpha$, we get $B T_{x=1} = \lambda_1^{-1} ((\lambda_1 v_1 - \lambda_2 \alpha v_2)^2 - v_2^2 (\alpha^2 \lambda_2^2 + \lambda_2 \lambda_1)) > 0$, since $\alpha^2 \lambda_2^2 + \lambda_2 \lambda_1 = 2((\sqrt{2} - 1)^2 - 1) < 0$. By applying the characteristic boundary conditions we obtain the following energy estimate:

$$\frac{d}{dt} \|v\|^2 = v^T \Omega_0 v|_{x=0} - v^T \Omega_1 v|_{x=1} + \eta \|v\|^2 + \frac{1}{\eta} \|F\|^2 - 2 \int_0^1 v_x^T \tilde{D} v_x \, dx, \quad (39)$$

where the matrix Ω_0 is negative definite and Ω_1 is positive definite

$$\Omega_0 = \begin{bmatrix} -\lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}, \quad \Omega_1 = \begin{bmatrix} \lambda_1 & -\alpha\lambda_2 \\ -\alpha\lambda_2 & -\lambda_2 \end{bmatrix}. \quad (40)$$

4.2.2. The semidiscrete problem

When analyzing system of equations it is convenient to introduce the *Kronecker product*,

$$C \otimes D = \begin{bmatrix} c_{0,0}D & \cdots & c_{0,q-1}D \\ \vdots & & \vdots \\ c_{p-1,0}D & \cdots & c_{p-1,q-1}D \end{bmatrix},$$

where C is a $p \times q$ matrix and D is a $m \times n$ matrix. Two useful rules for the Kronecker product are $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$, and $(A \otimes B)^T = A^T \otimes B^T$.

Before we proceed by constructing the semidiscrete approximation we write the boundary operators (see (36)) in matrix notation

$$\begin{aligned} L_0 &= I_0 A + (I_1 - I_0) \tilde{D} \frac{\partial}{\partial x}, \\ L_1 &= I_1 A + (I_0 - (I_2 + \alpha I_R) I_1) \tilde{D} \frac{\partial}{\partial x}, \end{aligned} \quad (41)$$

where

$$I_0 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad I_1 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad I_R = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Remark. In (41) we have included the discrete version of the relation $G_1 = \alpha G_2$, necessary for stability reasons in the discrete case. The relation $G_1 = \alpha G_2$ is not a regular boundary condition, it can be considered as a compatibility relation or a numerical boundary condition.

The corresponding boundary operators in the semidiscrete approximation become

$$\begin{aligned} \bar{L}_0 &= I_0 A \otimes E_0 + (I_1 - I_0) \tilde{D} \otimes E_0 S, \\ \bar{L}_1 &= I_1 A \otimes E_N + (I_0 - (I_2 + \alpha I_R) I_1) \tilde{D} \otimes E_N S. \end{aligned} \quad (42)$$

Note that the matrix S corresponds to the boundary derivative operator (see Section 2.2). The SAT method applied to (36) leads to

$$\begin{aligned} v_t + [A \otimes H^{-1} Q] v &= [\tilde{D} \otimes H^{-1} (-A + BS)] v + F + \Sigma_0 \otimes H^{-1} \{ \bar{L}_0 v - g_0 \otimes e_0 \} \\ &\quad + \Sigma_1 \otimes H^{-1} \{ \bar{L}_1 v - g_1 \otimes e_N \} \end{aligned} \quad (43)$$

$$v(0) = f,$$

where $v^T = [v_0^{(1)}, v_1^{(1)}, \dots, v_N^{(1)}, v_0^{(2)}, v_1^{(2)}, \dots, v_N^{(2)}]$. E_0 , e_0 , E_N and e_N are defined in (1). The 2×2 -matrices Σ_0 and Σ_1 can be tuned in order to give a stable scheme.

Applying the energy method by multiplying (43) by $v^T(I_2 \otimes H)$, adding the transpose and making use of $Q + Q^T = B$ yields

$$\begin{aligned} \frac{d}{dt} \|v\|_H^2 \leq & v_0^T [A + 2\Sigma_0 I_0 A] v_0 + v_N^T [-A + 2\Sigma_1 I_1 A] v_N - 2v_0^T [I_2 - \Sigma_0(I_1 - I_0)] \tilde{D}(Sv)_0 \\ & + 2v_N^T [I_2 + \Sigma_1(I_0 - (I_2 + \alpha I_R)I_1)] \tilde{D}(Sv)_N + \eta \|v\|_H^2 + \frac{1}{\eta} \|F\|_H^2 - v^T (\tilde{D} \otimes (A + A^T)) v, \end{aligned} \tag{44}$$

where the notations $v_0^T = [v_0^{(1)}, v_0^{(2)}]$, $v_N^T = [v_N^{(1)}, v_N^{(2)}]$ have been used. $I_2 - \Sigma_0(I_1 - I_0) = 0$ and $I_2 + \Sigma_1(I_0 - (I_2 + \alpha I_R)I_1) = 0$, i.e.,

$$\Sigma_0 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \Sigma_1 = \begin{bmatrix} -1 & \alpha \\ 0 & 1 \end{bmatrix} \tag{45}$$

is required to bound the energy. Inserting (45) into (44) yields

$$\frac{d}{dt} \|v\|_H^2 = v_0^T \Omega_0 v_0 - v_N^T \Omega_1 v_N + \eta \|v\|_H^2 + \frac{1}{\eta} \|F\|_H^2 - v^T (\tilde{D} \otimes (A + A^T)) v. \tag{46}$$

The estimate (46) is an analog to the continuous energy estimate (39).

Remark. Without introducing the numerical boundary condition $G_1 = \alpha G_2$ at $x = 1$, the relation $I_2 + \Sigma_1(I_0 - (I_2 + \alpha I_R)I_1) = 0$ changes to $I_2 - \Sigma_1 I_1 = 0$, with no solution. Hence, the numerical boundary condition $G_1 = \alpha G_2$ is indeed necessary in order to get an energy estimate for the semidiscrete approximation of (36).

4.2.3. Numerical results

To test the accuracy of the approximation (43) of the incompletely parabolic system (36) we choose an analytic solution

$$v = \begin{bmatrix} -\sin(w(x - ct))e^{-bx} \\ \sin(w(x + ct))e^{-bx} \end{bmatrix},$$

and modify f , F and the boundary data accordingly. The convergence studies for the fourth and sixth order case are shown in Tables 5 and 6, where the convective terms have been treated with one order less accurate boundary closures, compared to the internal order of accuracy. The viscous terms in the $(2p)$ th order case are closed at the boundaries with stencils of order $2p - 2$ and $2p - 1$, and the corresponding boundary derivatives are approximated to $(2p - 1)$ th and $(2p)$ th order. Again we have included computations where the stability conditions (45) are violated by choosing $\Sigma_0 = 1/2 \text{diag}(-1, 1)$. In the computations presented in Tables 5–7 we have chosen $w = 10$, $b = 1$, $c = 1$, $\epsilon = 1$. The solutions are advanced in time using the standard fourth order Runge–Kutta method.

The numerical studies indicate that a difference approximation, with boundary closures two orders less accurate for the approximation of the second derivative (the hyperbolic approximation has one order less accurate boundary closures), and a physical boundary condition one order less accurate, compared to the internal accuracy, maintains the design order of accuracy. If the stability condition (45) is violated, the overall convergence rate is reduced by one order.

For the parabolic scalar equation we have shown that we can lower the accuracy by two orders, compared to the internal scheme, also for the approximation of the first derivative. This is the case when using a scheme based on the fourth order diagonal norm. However, for the incompletely parabolic system, the results for the fourth order diagonal norm approximation (Table 7) show that a second order less accurate boundary closure, compared to the internal scheme, for the approximation of the first derivative is not

Table 5
 $\log(l_2\text{-error})$ and convergence rate in the fourth order case, based on the block norm

N	l_2	q	l_2^v	q^v
(a) Second order boundary closure ^a				
30	-3.31		-3.26	
60	-4.52	3.91	-4.25	3.24
90	-5.23	4.00	-4.81	3.10
120	-5.74	4.03	-5.19	3.05
150	-6.13	4.03	-5.49	3.03
(b) Third order boundary closure				
30	-3.31		-3.27	
60	-4.50	3.84	-4.43	3.76
90	-5.21	3.97	-5.12	3.88
120	-5.71	4.00	-5.61	3.91
150	-6.10	4.01	-6.00	3.93

In the computations marked v , (45) is violated by choosing $\Sigma_0 = 1/2\text{diag}(-1, 1)$.

^a Note the loss of convergence.

Table 6
 $\log(l_2\text{-error})$ and convergence rate in the sixth order case, based on the block norm

N	l_2	q	l_2^v	q^v
(a) Fourth order boundary closure ^a				
30	-4.75		-4.57	
60	-6.66	6.20	-6.05	4.79
90	-7.72	5.94	-6.92	4.91
120	-8.48	6.01	-7.55	4.96
150	-9.07	6.00	-8.03	4.95
(b) Fifth order boundary closure				
30	-4.76		-4.72	
60	-6.66	6.16	-6.72	6.48
90	-7.72	5.93	-7.79	6.03
120	-8.48	6.02	-8.55	5.97
150	-9.07	6.05	-9.13	5.98

In the computations marked v , (45) is violated by choosing $\Sigma_0 = 1/2\text{diag}(-1, 1)$.

^a Note the loss of convergence.

Table 7
 $\log(l_2\text{-error})$ and convergence rate in the fourth order case, based on the diagonal norm, with second order boundary closure for both the first and the second derivative approximations

N	l_2	q
30	-2.59	
60	-3.61	3.33
90	-4.18	3.19
120	-4.58	3.13
150	-4.88	3.11
30	-2.60	
60	-3.55	3.10
90	-4.10	3.05
120	-4.48	3.05
150	-4.78	3.04

In the computations marked v , (45) is violated by choosing $\Sigma_0 = 1/2\text{diag}(-1, 1)$.

enough to maintain the accuracy of the internal scheme, even if (45) holds. In fact we can prove (see Appendix B) the following proposition.

Proposition 4.1. *Consider the incompletely parabolic system (33) with the boundary conditions (41) and the corresponding semidiscrete problem (43). If Assumption B.2 holds, Lemma 2 holds for both the hyperbolic part and the parabolic part of the error equation (see the remark in Appendix B)) and Lemma B.1 holds, then*

$$\|e\|_H = \mathcal{O}(h^{2p}). \quad (47)$$

We summarize the results for the incompletely parabolic system. The numerical studies indicate and it is proven in Appendix B, that a difference approximation for an incompletely parabolic system retain the design order of accuracy if an energy estimate exists and

- two orders less accurate boundary closures are used, compared to the internal accuracy, in the second derivative approximations;
- one orders less accurate boundary closures are used, compared to the internal accuracy, in the first derivative approximations;
- the physical boundary conditions are approximated with one order less accurate approximations, compared to the internal accuracy.

5. Conclusions

The main objective was to construct second derivative approximations that combined the following desirable properties:

- Stability for general parabolic and incompletely parabolic problems.
- High order of accuracy, preservation of the overall convergence rate.
- Maintaining simplicity of the numerical scheme.

To achieve the three properties above, we have constructed finite difference approximations for the second derivative with the requirements: (i) They satisfy a summation by parts rule based on the same norm as the existing first derivative SBP operator. (ii) They have a boundary closure which is at most two orders lower, compared to the internal accuracy of the scheme. (iii) They are of minimal width in the interior, i.e., the same width as the corresponding first derivative approximation.

Accuracy requirements for hyperbolic, parabolic and incompletely parabolic problems were studied. The error analysis showed and the numerical computations indicated that the second derivative operator can be closed with boundary approximations two orders less accurate, compared to the design order of the scheme, and still maintain the internal accuracy. One order less accurate approximations, compared to the internal accuracy, of the physical boundary conditions were also allowed.

The numerical tests indicated that there is a close connection between the overall convergence rate and the stability estimate. If the stability conditions were violated, the overall convergence rate was reduced by one order when using a second derivative approximation with two orders less accurate boundary closures.

Appendix A. A remark on the wave equation

We briefly consider the wave equation, since it introduces an extra stability requirement on the SBP operator (see also [2]). The energy method applied to the wave equation, $u_{tt} = u_{xx}$, leads to

$$\frac{d}{dt} \left(\|u_t\|^2 + \|u_x\|^2 \right) = 2u_t u_x|_0.$$

An energy estimate requires appropriate boundary conditions

$$\alpha u(0, t) + u_x(0, t) = g_0(t), \quad \beta u(1, t) + u_x(1, t) = g_1(t). \quad (\text{A.1})$$

Assuming that $g_0 = g_1 = 0$, the energy method leads to

$$\frac{d}{dt} \left(\|u_t\|^2 + \|u_x\|^2 + \beta u^2(1, t) - \alpha u^2(0, t) \right) = 0.$$

The problem has an energy estimate if

$$\alpha \leq 0, \quad \beta \geq 0. \quad (\text{A.2})$$

The semidiscrete approximation of the wave equation is

$$v_{tt} = H^{-1}(A + BS)v + \tau_l H^{-1}E_0(\alpha + S)v + \tau_r H^{-1}E_N(\beta + S)v, \quad (\text{A.3})$$

where the SAT method has been used to implement the (homogeneous) boundary conditions. E_0 and E_N are defined in (1). By choosing the penalty parameters as,

$$\tau_l = 1, \quad \tau_r = -1, \quad (\text{A.4})$$

we end up with $v_{tt} = -H^{-1}(A + C)v$, where $C = -\alpha E_0 + \beta E_N = C^T$. If (A.2) holds, C is positive semidefinite.

Lemma A.1. *If (A.2) and (A.4) hold, (A.3) has a non-growing solution if A is symmetric and positive semidefinite.*

Proof. If (A.2) and (A.4) hold, (A.3) can be written $v_{tt} = -H^{-1}(A + C)v$, where $C = C^T \geq 0$. To guarantee a non-growing solution, the eigenvalues of $-H^{-1}(A + C)$ must be non-positive and real. If A is symmetric and positive semidefinite this is guaranteed, since the eigenvalue problem $-H^{-1}(A + C)x = \lambda x$ can be written as the *symmetric-definite generalized eigen-problem* $-(A + C)x = \lambda Hx$, for which it can be shown (see for example [6]) that $\lambda_i = b_i/h_i$, where b_i are the eigenvalues to $-(A + C)$ and h_i are the eigenvalues to H . With $A = A^T \geq 0$, $b_i \leq 0$ and real. Since $H = H^T > 0$, this implies that also $\lambda_i \leq 0$ and real. \square

Due to Lemma A.1 we introduce yet another definition (compare with Definitions 1 and 2).

Definition A.2. A difference operator $H^{-1}(-A + BS)$ approximating $\partial^2/\partial x^2$ is said to be a symmetric second derivative SBP operator if it is an SBP operator and if $A = A^T$.

Hence, symmetric second derivative SBP operators (see Definition A.2) guarantee stable semidiscrete approximations to the wave equation, assuming that the boundary conditions are treated correctly.

Remark. The minimal width SBP operators in the full norm cases have non-symmetric $A : s$, which means that $H^{-1}(A + C)$ might have eigenvalues with an imaginary part. However, the minimal width SBP operators in the diagonal norm cases are symmetric second derivative SBP operators.

Appendix B. Error analysis

The analysis is more transparent if we transform the problem (36) back to the original form (33). We begin by transforming the boundary operators (41) back to the original variables, resulting in

$$\begin{aligned} \tilde{L}_0 &= I_0 RC + (I_1 - I_0) RD \frac{\partial}{\partial x}, \\ \tilde{L}_1 &= I_1 RC + (I_0 - (I_2 + \alpha I_R) I_1) RD \frac{\partial}{\partial x}. \end{aligned} \quad (\text{B.1})$$

The corresponding boundary operators in the semidiscrete approximation become

$$\begin{aligned} \tilde{\tilde{L}}_0 &= I_0 RC \otimes E_0 + (I_1 - I_0)RD \otimes E_0 S, \\ \tilde{\tilde{L}}_1 &= I_1 RC \otimes E_N + (I_0 - (I_2 + \alpha I_R)I_1)RD \otimes E_N S. \end{aligned} \tag{B.2}$$

The semidiscrete approximation is given by

$$\begin{aligned} u_t + [C \otimes H^{-1}Q]u &= [D \otimes H^{-1}(-A + BS)]u + F + \Gamma_0 \otimes H^{-1} \left\{ \tilde{\tilde{L}}_0 u - g_0 \otimes e_0 \right\} \\ &\quad + \Gamma_1 \otimes H^{-1} \left\{ \tilde{\tilde{L}}_1 u - g_1 \otimes e_N \right\}, \\ u(0) &= f, \end{aligned} \tag{B.3}$$

where Γ_0 and Γ_1 are the transformed penalty matrices. The transformed stability conditions are

$$\Gamma_0 = R^T \Sigma_0, \quad \Gamma_1 = R^T \Sigma_1, \tag{B.4}$$

where Σ_0 and Σ_1 are given in (45) and R is given in (34).

Only the second equation has contributions from the second derivative approximation. However, it is not clear whether the first equation contain contributions from the boundary derivative approximations, coming from the penalty terms. Before we proceed we note that

$$\begin{aligned} \Gamma_0(I_0 - I_1)RD &= -D, \quad \Gamma_0 I_0 RC = P^{(0)}, \\ \Gamma_1(I_0 - (I_2 + \alpha I_R)I_1)RD &= -D, \quad \Gamma_1 I_1 RC = P^{(1)}, \end{aligned}$$

where

$$P^{(0)} = -\frac{1}{2} \begin{bmatrix} \sqrt{2} + 1 & 1 \\ 1 & \sqrt{2} - 1 \end{bmatrix}, \quad P^{(1)} = \sqrt{2} \begin{bmatrix} 0 & 0 \\ \sqrt{2} - 1 & -1 \end{bmatrix}.$$

We are interested in the error $e_j(t) = u(x_j, t) - v_j(t)$ and the error equation is given by

$$e_t - Me = T, \tag{B.5}$$

where

$$M = \begin{bmatrix} H^{-1}(Q - P_{1,1}^{(0)}E_0) & H^{-1}(Q - P_{1,2}^{(0)}E_0) \\ H^{-1}(Q - P_{2,1}^{(0)}E_0 - P_{2,1}^{(1)}E_1) & M_{2,2} \end{bmatrix},$$

$$M_{2,2} = -H^{-1}(Q + P_{2,2}^{(0)}E_0 + P_{2,2}^{(1)}E_1 - \epsilon(-A + BS) - \epsilon E_0 S + \epsilon E_1 S),$$

$T^T = [T^{(1)}, T^{(2)}]$ is the truncation error, with contributions from the approximation of the derivatives and the approximation of the boundary derivatives (Su) in the penalty terms. The structure of the problem shows that only the block $M_{2,2}$ contains the second and boundary derivative approximations. This means that $T^{(1)}$ will have contributions only from the first derivative approximation.

Remark. Note that $e_t^{(1)} - M_{1,1}e^{(1)}$ corresponds to the left-hand side of the error equation (18) emerging from a stable approximation of $u_t + u_x = 0$ with $u = g(t)$ on the left boundary. Also note that $e_t^{(2)} - M_{2,2}e^{(2)}$ corresponds to the left-hand side of the error equation (18) emerging from a stable approximation of the advection–diffusion equation (13) with $a = -1$, $\alpha = \frac{1-\sqrt{2}}{2\epsilon}$, $\beta = \frac{\sqrt{2}}{\epsilon}$.

As before we split the error and the truncation error into two parts, $e = e_i + e_b$ and $T = T_i + T_b$. The internal truncation error T_i is of order $\mathcal{O}(h^{2p})$. T_i and T_b have the structure shown in (20).

Lemma B.1. *If (B.4) holds for the penalty matrices in (B.3), then*

$$\|e_i\|_H \leq \mathcal{O}(h^{2p}). \quad (\text{B.6})$$

Proof. The energy method applied to the inner part of the error leads to

$$\|e_i\|_H \leq \frac{\exp(\frac{M}{2})}{\sqrt{\eta}} (\|T_i\|_H)_{\max(0,t)} = \mathcal{O}(h^{2p})$$

(where η is an arbitrary positive constant) if (B.4) holds. \square

To estimate e_b (to simplify notation we skip the subscripts in e_b and T_b) we use the Laplace transform technique, i.e.

$$(S \otimes I_N) \hat{e} - M \hat{e} = T, \quad (\text{B.7})$$

where $\hat{e} = [\hat{e}^{(1)}, \hat{e}^{(2)}]^T$, $S = \text{diag}(s, s)$ and I_N is the identity matrix. We multiply (B.7) by $(\text{diag}(h, h^2) \otimes I_N)$ and end up with

$$P \hat{e} = \tilde{T}, \quad (\text{B.8})$$

where $P = (\tilde{S} \otimes I_N - \tilde{M})$, $\tilde{S} = \text{diag}(sh, sh^2) = \text{diag}(\tilde{s}, \tilde{s})$ and $\tilde{T} = [\tilde{T}^{(1)}, \tilde{T}^{(2)}] = [hT^{(1)}, h^2T^{(2)}]$. Note that $P_{2,1}$ is of order $\mathcal{O}(h)$.

Remark. A necessary requirement (as will be shown in proof of Proposition 4.1) in order to obtain a $(2p)$ th order accurate difference approximation of an incompletely parabolic system is that $hT^{(1)} = h^2T^{(2)} = \mathcal{O}(h^{2p})$. This shows that the first derivative approximation needs to be $(2p-1)$ th order accurate at the boundaries, and that the second order derivative approximation needs to be $(2p-2)$ th order accurate at the boundaries.

We need the following assumption.

Assumption B.2. The solution to (B.8) can be expanded in a power series, i.e.

$$\hat{e} = \sum_{j=0}^{\infty} \hat{e}_j h^j. \quad (\text{B.9})$$

Remark. In the following proof of Proposition 4.1, $P_{1,1} \hat{e}^{(1)} = \tilde{T}^{(1)}$ (where $\tilde{T}^{(1)}$ is of order $\mathcal{O}(h^{2p})$) will be referred to as the hyperbolic part of the error equation since it corresponds to (23), emerging from a stable approximation of (5). Similarly $P_{2,2} \hat{e}^{(2)} = \tilde{T}^{(2)}$ (where $\tilde{T}^{(2)}$ is of order $\mathcal{O}(h^{2p})$) will be referred to as the parabolic part of the error equation since it corresponds to the error equation (23) emerging from a stable approximation of the advection–diffusion equation (13) with $a = -1$, $\alpha = \frac{1-\sqrt{2}}{2c}$, $\beta = \frac{\sqrt{2}}{c}$.

In the following proof, we consider the original form (33) of the system, i.e., with the boundary operators (B.1) and the corresponding semidiscrete problem (B.3).

Proof of Proposition 4.1. By inserting (B.9) in (B.8), and denoting $P_{2,1} = h\tilde{P}_{2,1}$ we get

$$\begin{bmatrix} P_{1,1} & P_{1,2} \\ 0 & P_{2,2} \end{bmatrix} \begin{bmatrix} \hat{e}_0^{(1)} \\ \hat{e}_0^{(2)} \end{bmatrix} = \begin{bmatrix} \tilde{T}^{(1)} \\ \tilde{T}^{(2)} \end{bmatrix} \tag{B.10}$$

for the leading order terms (i.e., $\hat{e}_0^{(1)}$ and $\hat{e}_0^{(2)}$).

Remark. Note that \tilde{T} in (B.8) is of $\mathcal{O}(h^{2p})$, and that the leading order terms in fact are of order $2p$. This is only a matter of normalization.

The equations for the higher order terms are given by the following recursion formula:

$$\begin{bmatrix} P_{1,1} & P_{1,2} \\ 0 & P_{2,2} \end{bmatrix} \begin{bmatrix} \hat{e}_p^{(1)} \\ \hat{e}_p^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ -\tilde{P}_{2,1}\hat{e}_{p-1}^{(1)} \end{bmatrix}, \quad p = 1, 2, \dots \tag{B.11}$$

This indicates that (B.9) is a reasonable assumption.

The second row in (B.10) yields $P_{2,2}\hat{e}_0^{(2)} = \tilde{T}^{(2)}$. Recall that $\tilde{T}^{(2)}$ is zero in the interior. If Lemma 2 holds for the parabolic part, then $\hat{e}_0^{(2)} = \mathcal{O}(h^{2p})$. By using Parsevals relation we obtain $e_b^{(2)}(t) = \mathcal{O}(h^{2p})$ (here the subscript b is reintroduced to elucidate that we only include the boundary part). From (B.6) we obtain $e^{(2)}(t) = e_i^{(2)} + e_b^{(2)} = \mathcal{O}(h^{2p})$.

We now return to the error Eq. (B.5) and consider the first row, $e_t^{(1)} - M_{1,1}e^{(1)} = M_{1,2}e^{(2)} + T^{(1)}$. Note that $e^{(1)}, e^{(2)}$ and $T^{(1)}$ now include both the interior and the boundary parts. Since $e^{(2)}$ is estimated we can introduce $\tilde{T}^{(1)} = M_{1,2}e^{(2)} + T^{(1)}$ as a modified truncation error, i.e., $e_t^{(1)} - M_{1,1}e^{(1)} = \tilde{T}^{(1)}$, where $\tilde{T}^{(1)}$ has the structure of (19) with $r = 2p - 1$. Again the error and the truncation error are split into two parts $e^{(1)} = e_i^{(1)} + e_b^{(1)}$ and $\tilde{T}^{(1)} = \tilde{T}_i^{(1)} + \tilde{T}_b^{(1)}$, where the internal truncation error $\tilde{T}_i^{(1)}$ is of order $\mathcal{O}(h^{2p})$. Since $e_t^{(1)} - M_{1,1}e^{(1)} = \tilde{T}^{(1)}$ corresponds to the error equation emerging from a stable approximation of $u_t + u_x = 0$ with $u = g(t)$ on the left boundary, the energy estimate leads to $\|e_i^{(1)}\|_H \leq \mathcal{O}(h^{2p})$.

To estimate $e_b^{(1)}$ we again use the Laplace transform technique, which leads to $P_{1,1}\hat{e}_b^{(1)} = h\tilde{T}_b^{(1)}$ (where $h\tilde{T}_b^{(1)}$ is of order $\mathcal{O}(h^{2p})$). If Lemma 2 holds for the hyperbolic part, then $\hat{e}_b^{(1)} = \mathcal{O}(h^{2p})$ and we obtain $e^{(1)}(t) = e_i^{(1)} + e_b^{(1)} = \mathcal{O}(h^{2p})$. This completes the proof. \square

Appendix C. Diagonal norms

We now present the SBP operators used in the analysis, based on diagonal norms. We consider second, third, fourth and fifth order accurate finite difference approximations.

C.1. First order accuracy at the boundary

The discrete norm H and the discrete second order accurate SBP operator $H^{-1}Q$ approximating $\frac{d}{dx}$ are given by

$$H = h \begin{bmatrix} \frac{1}{2} & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & \frac{1}{2} \end{bmatrix}, \quad H^{-1}Q = \frac{1}{h} \begin{bmatrix} -1 & 1 & & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{2} & 0 & \frac{1}{2} \\ & & & -1 & 1 \end{bmatrix}.$$

The discrete second order accurate SBP operator $D_2 = H^{-1}(-A + BS)$ approximating $\frac{d^2}{dx^2}$ and the boundary derivative operator BS are given by

$$D_2 = \frac{1}{h^2} \begin{bmatrix} 1 & -2 & 1 & & & & \\ 1 & -2 & 1 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & & 1 & -2 & 1 & \\ & & & 1 & -2 & 1 & \end{bmatrix}, \quad BS = \frac{1}{h} \begin{bmatrix} \frac{3}{2} & -2 & \frac{1}{2} & & & & \\ & 1 & & & & & \\ & & \ddots & & & & \\ & & & & 1 & & \\ & & & \frac{1}{2} & -2 & \frac{3}{2} & \end{bmatrix}.$$

C.2. Second order accuracy at the boundary

The discrete norm H is defined as

$$H = h \begin{bmatrix} \frac{17}{48} & & & & & & \\ & \frac{59}{48} & & & & & \\ & & \frac{43}{48} & & & & \\ & & & \frac{49}{48} & & & \\ & & & & 1 & & \\ & & & & & \ddots & \\ & & & & & & \ddots \end{bmatrix}.$$

The discrete difference SBP operator approximating $\frac{d}{dx}$ we denote $D_1 = H^{-1}Q$.

$$D_1 = \frac{1}{h} \begin{bmatrix} -\frac{24}{17} & \frac{59}{34} & -\frac{4}{17} & -\frac{3}{34} & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ \frac{4}{43} & -\frac{59}{86} & 0 & \frac{59}{86} & -\frac{4}{43} & 0 & 0 \\ \frac{3}{98} & 0 & -\frac{59}{98} & 0 & \frac{32}{49} & -\frac{4}{49} & 0 \\ 0 & 0 & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} \\ & & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

The discrete fourth order accurate SBP operator $D_2 = H^{-1}(-A + BS)$ approximating $\frac{d^2}{dx^2}$ is given by

$$D_2 = \frac{1}{h^2} \begin{bmatrix} 2 & -5 & 4 & -1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ -\frac{4}{43} & \frac{59}{43} & -\frac{110}{43} & \frac{59}{43} & -\frac{4}{43} & 0 & 0 \\ -\frac{1}{49} & 0 & \frac{59}{49} & -\frac{118}{49} & \frac{64}{49} & -\frac{4}{49} & 0 \\ 0 & 0 & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & \frac{1}{12} \\ & & & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

and the third order accurate boundary derivative operator BS is given by,

$$BS = \frac{1}{h} \begin{bmatrix} \frac{11}{6} & -3 & \frac{3}{2} & -\frac{1}{3} \\ & 0 & & \\ & & \ddots & \\ & & & 0 \\ & -\frac{1}{3} & \frac{3}{2} & -3 & \frac{11}{6} \end{bmatrix}.$$

C.3. Third order accuracy at the boundary

The discrete norm H is defined as

$$H = h \begin{bmatrix} \frac{13649}{43200} & & & & & & & & & & \\ & \frac{12013}{8640} & & & & & & & & & \\ & & \frac{2711}{4320} & & & & & & & & \\ & & & \frac{5359}{4320} & & & & & & & \\ & & & & \frac{7877}{8640} & & & & & & \\ & & & & & \frac{43801}{43200} & & & & & \\ & & & & & & 1 & & & & \\ & & & & & & & \ddots & & & \\ & & & & & & & & \ddots & & \end{bmatrix}.$$

The discrete difference operator approximating $\frac{d}{dx}$ we denote (here) $D_1 = H^{-1}Q$, obeying our wanted SBP property

$$D1 = \frac{1}{h} \begin{bmatrix} -\frac{21600}{13649} & \frac{104009}{54596} & \frac{30443}{81894} & -\frac{33311}{27298} & \frac{16863}{27298} & -\frac{15025}{163788} & 0 & 0 & 0 & 0 \\ -\frac{104009}{240260} & 0 & -\frac{311}{72078} & \frac{20229}{24026} & -\frac{24337}{48052} & \frac{36661}{360390} & 0 & 0 & 0 & 0 \\ -\frac{30443}{162660} & \frac{311}{32532} & 0 & -\frac{11155}{16266} & \frac{41287}{32532} & -\frac{21999}{54220} & 0 & 0 & 0 & 0 \\ \frac{33311}{107180} & -\frac{20229}{21436} & \frac{485}{1398} & 0 & \frac{4147}{21436} & \frac{25427}{321540} & \frac{72}{5359} & 0 & 0 & 0 \\ -\frac{16863}{78770} & \frac{24337}{31508} & -\frac{41287}{47262} & -\frac{4147}{15754} & 0 & \frac{342523}{472620} & -\frac{1296}{7877} & \frac{144}{7877} & 0 & 0 \\ \frac{15025}{525612} & -\frac{36661}{262806} & \frac{21999}{87602} & -\frac{25427}{262806} & -\frac{342523}{525612} & 0 & \frac{32400}{43801} & -\frac{6480}{43801} & \frac{720}{43801} & 0 \\ 0 & 0 & 0 & -\frac{1}{60} & \frac{3}{20} & -\frac{3}{4} & 0 & \frac{3}{4} & -\frac{3}{20} & \frac{1}{60} \\ & & & & & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

The discrete difference operator approximating $\frac{d^2}{dx^2}$ obeying our wanted SBP property is written $D_2 = H^{-1}(-A + BS)$, where $A = A^T \leq 0$. The interior stencil is the standard sixth order accurate central scheme $h^2(D_2 v)_j = \frac{1}{90}v_{j-3} - \frac{3}{20}v_{j-2} + \frac{3}{2}v_{j-1} - \frac{49}{18}v_j + \frac{3}{2}v_{j+1} - \frac{3}{120}v_{j+2} + \frac{1}{90}v_{j+3}$. At the boundary the operator becomes

$$D2 = \frac{1}{h^2} \begin{bmatrix} \frac{114170}{40947} & -\frac{438107}{54596} & \frac{336409}{40947} & -\frac{276997}{81894} & \frac{3747}{13649} & \frac{21035}{163788} & 0 & 0 & 0 & 0 \\ \frac{6173}{5860} & -\frac{2066}{879} & \frac{3283}{1758} & -\frac{303}{293} & \frac{2111}{3516} & -\frac{601}{4395} & 0 & 0 & 0 & 0 \\ -\frac{52391}{81330} & \frac{134603}{32532} & -\frac{21982}{2711} & \frac{112915}{16266} & -\frac{46969}{16266} & \frac{30409}{54220} & 0 & 0 & 0 & 0 \\ \frac{68603}{321540} & -\frac{12423}{10718} & \frac{112915}{32154} & -\frac{75934}{16077} & \frac{53369}{21436} & -\frac{54899}{160770} & \frac{48}{5359} & 0 & 0 & 0 \\ -\frac{7053}{39385} & \frac{86551}{94524} & -\frac{46969}{23631} & \frac{53369}{15754} & -\frac{87904}{23631} & \frac{820271}{472620} & -\frac{1296}{7877} & \frac{96}{7877} & 0 & 0 \\ \frac{21035}{525612} & -\frac{24641}{131403} & \frac{30409}{87602} & -\frac{54899}{131403} & \frac{820271}{525612} & -\frac{117600}{43801} & \frac{64800}{43801} & -\frac{6480}{43801} & \frac{480}{43801} & 0 \\ 0 & 0 & 0 & \frac{1}{90} & -\frac{3}{20} & 3/2 & -\frac{49}{18} & 3/2 & -\frac{3}{20} & \frac{1}{90} \\ & & & & & & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

and the boundary derivative operator of fourth order accuracy is

$$BS = \frac{1}{h} \begin{bmatrix} \frac{25}{12} & -4 & 3 & -\frac{4}{3} & \frac{1}{4} \\ & & 0 & & \\ & & & \ddots & \\ & & & & 0 \\ & \frac{1}{4} & -\frac{4}{3} & 3 & -4 & \frac{25}{12} \end{bmatrix}.$$

C.4. Fourth order accuracy at the boundary

The discrete difference operator approximating $\frac{d}{dx}$ we denote (here) $D_1 = H^{-1}Q$, obeying our wanted SBP property

$$\begin{array}{llll} D_{1,1,1} = \frac{-2540160}{1498139} & D_{1,3,1} = \frac{-66264997}{8719620} & D_{1,5,1} = \frac{-20708767}{2096689} & D_{1,7,1} = \frac{-27390659}{56287644} \\ D_{1,1,2} = \frac{5544277}{5992556} & D_{1,3,2} = \frac{9444709}{415220} & D_{1,5,2} = 1 \frac{65990199}{3594324} & D_{1,7,2} = \frac{7568311}{2680364} \\ D_{1,1,3} = \frac{198794991}{29962780} & D_{1,3,3} = 0 & D_{1,5,3} = \frac{-96962637}{1198108} & D_{1,7,3} = \frac{-22524966}{3350455} \\ D_{1,1,4} = \frac{-256916579}{17977668} & D_{1,3,4} = \frac{-20335981}{249132} & D_{1,5,4} = \frac{68748371}{1198108} & D_{1,7,4} = \frac{66558305}{8041092} \\ D_{1,1,5} = \frac{20708767}{1498139} & D_{1,3,5} = \frac{32320879}{249132} & D_{1,5,5} = 0 & D_{1,7,5} = \frac{-14054993}{2680364} \\ D_{1,1,6} = \frac{-41004357}{5992556} & D_{1,3,6} = \frac{-35518713}{415220} & D_{1,5,6} = \frac{-27294549}{1198108} & D_{1,7,6} = \frac{2084949}{2680364} \\ D_{1,1,7} = \frac{27390659}{17977668} & D_{1,3,7} = \frac{2502774}{103805} & D_{1,5,7} = \frac{14054993}{1198108} & D_{1,7,7} = 0 \\ D_{1,1,8} = \frac{-2323531}{29962780} & D_{1,3,8} = \frac{-3177073}{1743924} & D_{1,5,8} = \frac{-42678199}{25160268} & D_{1,7,8} = \frac{70710683}{93812740} \\ D_{1,1,9} = 0 & D_{1,3,9} = 0 & D_{1,5,9} = \frac{-2592}{299527} & D_{1,7,9} = \frac{-145152}{670091} \\ D_{1,1,10} = 0 & D_{1,3,10} = 0 & D_{1,5,10} = 0 & D_{1,7,10} = \frac{27648}{670091} \\ D_{1,1,11} = 0 & D_{1,3,11} = 0 & D_{1,5,11} = 0 & D_{1,7,11} = -\frac{2592}{670091} \end{array}$$

$D1_{1,12} = 0$	$D1_{3,12} = 0$	$D1_{5,12} = 0$	$D1_{7,12} = 0$
$D1_{2,1} = \frac{-5544277}{31004596}$	$D1_{4,1} = \frac{256916579}{109619916}$	$D1_{6,1} = \frac{13668119}{8660148}$	$D1_{8,1} = \frac{2323531}{102554780}$
$D1_{2,2} = 0$	$D1_{4,2} = \frac{-49607267}{5219996}$	$D1_{6,2} = \frac{-850651}{103097}$	$D1_{8,2} = \frac{-48319961}{307664340}$
$D1_{2,3} = \frac{-85002381}{22146140}$	$D1_{4,3} = \frac{61007943}{5219996}$	$D1_{6,3} = \frac{35518713}{2061940}$	$D1_{8,3} = \frac{9531219}{20510956}$
$D1_{2,4} = \frac{49607267}{4429228}$	$D1_{4,4} = 0$	$D1_{6,4} = \frac{-21696041}{1237164}$	$D1_{8,4} = \frac{-3870214}{5127739}$
$D1_{2,5} = \frac{-165990199}{13287684}$	$D1_{4,5} = \frac{-68748371}{5219996}$	$D1_{6,5} = \frac{9098183}{1237164}$	$D1_{8,5} = \frac{2246221}{3238572}$
$D1_{2,6} = \frac{7655859}{1107307}$	$D1_{4,6} = \frac{65088123}{5219996}$	$D1_{6,6} = 0$	$D1_{8,6} = \frac{-21360021}{102554780}$
$D1_{2,7} = \frac{-7568311}{4429228}$	$D1_{4,7} = \frac{-66558305}{15659988}$	$D1_{6,7} = \frac{-231661}{412388}$	$D1_{8,7} = \frac{-70710683}{102554780}$
$D1_{2,8} = \frac{48319961}{465068940}$	$D1_{4,8} = \frac{3870214}{9134993}$	$D1_{6,8} = \frac{7120007}{43300740}$	$D1_{8,8} = 0$
$D1_{2,9} = 0$	$D1_{4,9} = 0$	$D1_{6,9} = \frac{3072}{103097}$	$D1_{8,9} = \frac{4064256}{5127739}$
$D1_{2,10} = 0$	$D1_{4,10} = 0$	$D1_{6,10} = \frac{-288}{103097}$	$D1_{8,10} = \frac{-1016064}{5127739}$
$D1_{2,11} = 0$	$D1_{4,11} = 0$	$D1_{6,11} = 0$	$D1_{8,11} = \frac{193536}{5127739}$
$D1_{2,12} = 0$	$D1_{4,12} = 0$	$D1_{6,12} = 0$	$D1_{8,12} = \frac{-18144}{5127739}$

In the interior we have the eighth order accurate central operator

$$h(D_1 v)_j = \frac{1}{280} v_{j-4} - \frac{4}{105} v_{j-3} + \frac{1}{5} v_{j-2} - \frac{4}{5} v_{j-1} + \frac{4}{5} v_{j+1} - \frac{1}{5} v_{j+2} + \frac{4}{105} v_{j+3} - \frac{1}{280} v_{j+4}.$$

The discrete difference operator approximating $\frac{d^2}{dx^2}$ obeying our wanted SBP property is written $D_2 = H^{-1}(-A + BS)$, where $A = A^T \geq 0$. The interior stencil is the standard eight order accurate central scheme

$$h^2(D_2v)_j = -\frac{1}{560}v_{j-4} + \frac{8}{315}v_{j-3} - \frac{1}{5}v_{j-2} + \frac{8}{5}v_{j-1} - \frac{205}{72}v_j + \frac{8}{5}v_{j+1} - \frac{1}{5}v_{j+2} + \frac{8}{315}v_{j+3} - \frac{1}{560}v_{j+4}.$$

At the boundary the operator becomes

$D_{2,1,1} = \frac{4870382994799}{1358976868290}$	$D_{2,3,1} = \frac{7838984095}{52731029988}$	$D_{2,5,1} = \frac{1455067816}{21132528431}$	$D_{2,7,1} = \frac{-135555328849}{8509847458140}$
$D_{2,1,2} = \frac{-893640087518}{75498714905}$	$D_{2,3,2} = \frac{1168338040}{5649753213}$	$D_{2,5,2} = \frac{-171562838}{3018932633}$	$D_{2,7,2} = \frac{11904122576}{101307707835}$
$D_{2,1,3} = \frac{926594825119}{60398971924}$	$D_{2,3,3} = \frac{-88747895}{144865467}$	$D_{2,5,3} = \frac{-43205598281}{36227191596}$	$D_{2,7,3} = \frac{-5124426509}{13507694378}$
$D_{2,1,4} = \frac{-1315109406200}{135897686829}$	$D_{2,3,4} = \frac{423587231}{627750357}$	$D_{2,5,4} = \frac{48242560214}{9056797899}$	$D_{2,7,4} = \frac{43556319241}{60784624701}$
$D_{2,1,5} = \frac{39126983272}{15099742981}$	$D_{2,3,5} = \frac{-43205598281}{22599012852}$	$D_{2,5,5} = \frac{-52276055645}{6037865266}$	$D_{2,7,5} = \frac{-80321706377}{81046166268}$
$D_{2,1,6} = \frac{12344491342}{75498714905}$	$D_{2,3,6} = \frac{4876378562}{1883251071}$	$D_{2,5,6} = \frac{57521587238}{9056797899}$	$D_{2,7,6} = \frac{73790130002}{33769235945}$
$D_{2,1,7} = \frac{-451560522577}{2717953736580}$	$D_{2,3,7} = \frac{-5124426509}{3766502142}$	$D_{2,5,7} = \frac{-80321706377}{36227191596}$	$D_{2,7,7} = \frac{-950494905688}{303923123505}$
$D_{2,1,8} = 0$	$D_{2,3,8} = \frac{10496900965}{39548272491}$	$D_{2,5,8} = \frac{8078087158}{21132528431}$	$D_{2,7,8} = \frac{239073018673}{141830790969}$
$D_{2,1,9} = 0$	$D_{2,3,9} = 0$	$D_{2,5,9} = \frac{-1296}{299527}$	$D_{2,7,9} = \frac{-145152}{670091}$
$D_{2,1,10} = 0$	$D_{2,3,10} = 0$	$D_{2,5,10} = 0$	$D_{2,7,10} = \frac{18432}{670091}$
$D_{2,1,11} = 0$	$D_{2,3,11} = 0$	$D_{2,5,11} = 0$	$D_{2,7,11} = \frac{-1296}{670091}$

$$\begin{array}{llll}
D2_{1,12} = 0 & D2_{3,12} = 0 & D2_{5,12} = 0 & D2_{7,12} = 0 \\
D2_{2,1} = \frac{333806012194}{390619153855} & D2_{4,1} = \frac{-94978241528}{828644350023} & D2_{6,1} = \frac{10881504334}{327321118845} & D2_{8,1} = 0 \\
D2_{2,2} = \frac{-154646272029}{111605472530} & D2_{4,2} = \frac{82699112501}{157837019052} & D2_{6,2} = \frac{-28244698346}{140280479505} & D2_{8,2} = \frac{-2598164715}{206729925524} \\
D2_{2,3} = \frac{1168338040}{33481641759} & D2_{4,3} = \frac{1270761693}{13153084921} & D2_{6,3} = \frac{4876378562}{9352031967} & D2_{8,3} = \frac{10496900965}{155047444143} \\
D2_{2,4} = \frac{82699112501}{133926567036} & D2_{4,4} = \frac{-167389605005}{118377764289} & D2_{6,4} = \frac{-10557998671}{12469375956} & D2_{8,4} = \frac{-44430275135}{310094888286} \\
D2_{2,5} = \frac{-171562838}{11160547253} & D2_{4,5} = \frac{48242560214}{39459254763} & D2_{6,5} = \frac{57521587238}{28056095901} & D2_{8,5} = \frac{425162482}{2720130599} \\
D2_{2,6} = \frac{-28244698346}{167408208795} & D2_{4,6} = \frac{-31673996013}{52612339684} & D2_{6,6} = \frac{-278531401019}{93520319670} & D2_{8,6} = \frac{-137529995233}{620189776572} \\
D2_{2,7} = \frac{11904122576}{167408208795} & D2_{4,7} = \frac{43556319241}{118377764289} & D2_{6,7} = \frac{73790130002}{46760159835} & D2_{8,7} = \frac{239073018673}{155047444143} \\
D2_{2,8} = \frac{-2598164715}{312495323084} & D2_{4,8} = \frac{-44430275135}{552429566682} & D2_{6,8} = \frac{-137529995233}{785570685228} & D2_{8,8} = \frac{-144648000000}{51682481381} \\
D2_{2,9} = 0 & D2_{4,9} = 0 & D2_{6,9} = \frac{2048}{103097} & D2_{8,9} = \frac{8128512}{5127739} \\
D2_{2,10} = 0 & D2_{4,10} = 0 & D2_{6,10} = \frac{-144}{103097} & D2_{8,10} = \frac{-1016064}{5127739} \\
D2_{2,11} = 0 & D2_{4,11} = 0 & D2_{6,11} = 0 & D2_{8,11} = \frac{129024}{5127739} \\
D2_{2,12} = 0 & D2_{4,12} = 0 & D2_{6,12} = 0 & D2_{8,12} = \frac{-9072}{5127739}
\end{array}$$

and the boundary derivative operator of fifth order accuracy

$$BS = \frac{1}{h} \begin{bmatrix} \frac{4723}{2100} & -\frac{839}{175} & \frac{157}{35} & -\frac{278}{105} & \frac{103}{140} & \frac{1}{175} & -\frac{6}{175} & & & & \\ & & & 0 & & & & & & & \\ & & & & \ddots & & & & & & \\ & & & & & 0 & & & & & \\ & & & -\frac{6}{175} & \frac{1}{175} & \frac{103}{140} & -\frac{278}{105} & \frac{157}{35} & -\frac{839}{175} & \frac{4723}{2100} & \\ & & & & & & & & & & \end{bmatrix}.$$

The discrete norm H is defined as

$$\begin{aligned}
 H_{1,1} &= \frac{1498139}{5080320} & H_{3,3} &= \frac{20761}{80640} & H_{5,5} &= \frac{299527}{725760} & H_{7,7} &= \frac{670091}{725760} \\
 H_{2,2} &= \frac{1107307}{725760} & H_{4,4} &= \frac{1304999}{725760} & H_{6,6} &= \frac{103097}{80640} & H_{8,8} &= \frac{5127739}{5080320}
 \end{aligned}$$

Appendix D. Full norms

We now present the SBP operators used in the analysis, based on full norms. We consider fourth, sixth and eighth order accurate finite difference approximations.

D.1. Fourth order accurate operators

We now present the specific form of the fourth order accurate operators used in the analysis. The discrete norm H is defined as

$$\begin{aligned}
 r1 &= -\frac{2177\sqrt{295369} - 1166427}{25488}, & r2 &= \frac{66195\sqrt{53}\sqrt{5573} - 35909375}{101952}, \\
 h11 &= -\frac{216r2 + 2160r1 - 2125}{12960}, & h23 &= \frac{1836r2 + 14580r1 + 7295}{2160}, \\
 h12 &= \frac{81r2 + 675r1 + 415}{540}, & h24 &= -\frac{216r2 + 2160r1 + 655}{4320}, \\
 h13 &= -\frac{72r2 + 720r1 + 445}{1440}, & h33 &= -\frac{4104r2 + 32400r1 + 12785}{4320}, \\
 h14 &= -\frac{108r2 + 756r1 + 421}{1296}, & h34 &= \frac{81r2 + 675r1 + 335}{540}, \\
 h22 &= -\frac{4104r2 + 32400r1 + 11225}{4320}, & h44 &= -\frac{216r2 + 2160r1 - 12085}{12960},
 \end{aligned}$$

At the boundary the operator with a second order boundary closure becomes

$$\begin{array}{lll} D2_{1,1} = 2.D0 & D2_{2,3} = 0.4451860342366326D0 & D2_{3,5} = -0.370366153552986D-2 \\ D2_{1,2} = -5.D0 & D2_{2,4} = 0.3889216118347602D0 & D2_{3,6} = -0.4126377895574793D-2 \\ D2_{1,3} = 4.D0 & D2_{2,5} = -0.1115146289530765D0 & D2_{4,1} = -0.1972518376035006D-1 \\ D2_{1,4} = -1.D0 & D2_{2,6} = 0.5713690397754591D-2 & D2_{4,2} = -0.3132697803201818D-2 \\ D2_{1,5} = 0.D0 & D2_{3,1} = -0.2020917311782903D-1 & D2_{4,3} = 0.1209782628816308D1 \\ D2_{1,6} = 0.D0 & D2_{3,2} = 0.1076710314575741D1 & D2_{4,4} = -0.2413299862026212D1 \\ D2_{2,1} = 0.9113401326379418D0 & D2_{3,3} = -0.2104749527124675D1 & D2_{4,5} = 0.1308408547618058D1 \\ D2_{2,2} = -0.1639646840154013D1 & D2_{3,4} = 0.1056078425097867D1 & D2_{4,6} = -0.8203343284460206D-1 \end{array}$$

and with a third order boundary derivative operator

$$BS = \frac{1}{h} \begin{bmatrix} \frac{11}{6} & -3 & \frac{3}{2} & -\frac{1}{3} & & & & & & \\ & & & 0 & & & & & & \\ & & & & \ddots & & & & & \\ & & & & & 0 & & & & \\ & & & & & & -\frac{1}{3} & \frac{3}{2} & -3 & \frac{11}{6} \end{bmatrix}.$$

D.2. Sixth order accurate operators

We now present the specific form of the sixth order accurate operators used in the analysis. The discrete norm H at the boundary is defined as

$$h11 = - \frac{14400 * r2 + 302400 * r1 - 7420003}{3.6288e7}$$

$$h12 = - \frac{75600 * r3 + 1497600 * r2 + 11944800 * r1 - 59330023}{2.17728e7}$$

$$h13 = - \frac{9450 * r3 + 202050 * r2 + 1776600 * r1 - 7225847}{340200.}$$

$$h14 = \frac{900 * r2 + 18900 * r1 - 649}{226800.}$$

$$h15 = \frac{86400 * r3 + 1828800 * r2 + 15854400 * r1 - 66150023}{3110400.}$$

$$h16 = \frac{378000 * r3 + 7747200 * r2 + 65167200 * r1 - 279318239}{1.08864e8}$$

$$h22 = \frac{302400 * r3 + 6091200 * r2 + 49896000 * r1 - 210294289}{7257600.}$$

$$h_{23} = \frac{3780 * r_3 + 82575 * r_2 + 741825 * r_1 - 2991977}{34020.}$$

$$h_{24} = \frac{5400 * r_3 + 104400 * r_2 + 810000 * r_1 - 3756643}{129600.}$$

$$h_{25} = -\frac{529200 * r_3 + 11107200 * r_2 + 95508000 * r_1 - 400851749}{2419200.}$$

$$h_{26} = \frac{86400 * r_3 + 1828800 * r_2 + 15854400 * r_1 - 65966279}{3110400.}$$

$$h_{33} = -\frac{51300 * r_3 + 1094400 * r_2 + 9585000 * r_1 - 39593423}{64800.}$$

$$h_{34} = \frac{120960 * r_3 + 2584800 * r_2 + 22680000 * r_1 - 93310367}{181440.}$$

$$h_{35} = \frac{5400 * r_3 + 104400 * r_2 + 810000 * r_1 - 3766003}{129600.}$$

$$h_{36} = \frac{900 * r_2 + 18900 * r_1 - 37217}{226800.}$$

$$h_{44} = -\frac{17100 * r_3 + 364800 * r_2 + 3195000 * r_1 - 13184701}{21600.}$$

$$h_{45} = \frac{3780 * r_3 + 82575 * r_2 + 741825 * r_1 - 2976857}{34020.}$$

$$h_{46} = -\frac{1890 * r_3 + 40410 * r_2 + 355320 * r_1 - 1458223}{68040.}$$

$$h_{55} = \frac{302400 * r_3 + 6091200 * r_2 + 49896000 * r_1 - 213056209}{7257600.}$$

$$h_{56} = -\frac{75600 * r_3 + 1497600 * r_2 + 11944800 * r_1 - 54185191}{2.17728e7}$$

$$h_{66} = -\frac{14400 * r_2 + 302400 * r_1 - 36797603}{3.6288e7}$$

where

$$r1 = -3.6224891259957,$$

$$r2 = 96.301901955532,$$

$$r3 = -609.05813881563.$$

The discrete sixth order accurate operator approximating $\frac{d}{dx}$ is denoted $H^{-1}Q$, obeying our wanted SBP property

$$Q = \begin{bmatrix} q_{11} & q_{12} & q_{13} & q_{14} & q_{15} & q_{16} & & & & & \\ -q_{12} & q_{22} & q_{23} & q_{24} & q_{25} & q_{26} & & & & & \\ -q_{13} & -q_{23} & q_{33} & q_{34} & q_{35} & q_{36} & & & & & \\ -q_{14} & -q_{24} & -q_{34} & q_{44} & q_{45} & q_{46} & q_3 & & & & \\ -q_{15} & -q_{25} & -q_{35} & -q_{45} & q_{55} & q_{56} & q_2 & q_3 & & & \\ -q_{16} & -q_{26} & -q_{36} & -q_{46} & -q_{56} & q_{66} & q_1 & q_2 & q_3 & & \\ & & & -q_3 & -q_2 & -q_1 & 0 & q_1 & q_2 & q_3 & \\ & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix},$$

where

$$q1 = \frac{1}{60}$$

$$q2 = \frac{9}{60}$$

$$q3 = \frac{45}{60}$$

$$q11 = \frac{-1.}{2}$$

$$q12 = \frac{415800 * r3 + 8604000 * r2 + 72954000 * r1 - 283104553}{3.26592e7}$$

$$q13 = \frac{120960 * r3 + 2672640 * r2 + 24192000 * r1 - 100358119}{6531840.}$$

$$q14 = -\frac{25200 * r3 + 542400 * r2 + 4788000 * r1 - 19717139}{403200.}$$

$$q15 = \frac{604800 * r3 + 13363200 * r2 + 120960000 * r1 - 485628701}{3.26592e7}$$

$$q_{16} = \frac{41580 * r_3 + 860400 * r_2 + 7295400 * r_1 - 31023481}{3265920.}$$

$$q_{22} = 0$$

$$q_{23} = -\frac{9450000 * r_3 + 200635200 * r_2 + 1747116000. * r_1 - 7286801279.}{3.26592e7}$$

$$q_{24} = \frac{21168000 * r_3 + 449049600 * r_2 + 3907008000. * r_1 - 16231108387.}{3.26592e7}$$

$$q_{25} = -\frac{165375 * r_3 + 3516300 * r_2 + 30665250 * r_1 - 126996371}{453600.}$$

$$q_{26} = \frac{604800 * r_3 + 13363200 * r_2 + 120960000. * r_1 - 482536157}{3.26592e7}$$

$$q_{33} = 0$$

$$q_{34} = -\frac{6993000 * r_3 + 148096800 * r_2 + 1286334000. * r_1 - 5353075351.}{8164800.}$$

$$q_{35} = \frac{21168000 * r_3 + 449049600 * r_2 + 3907008000. * r_1 - 16212561187.}{3.26592e7}$$

$$q_{36} = -\frac{75600 * r_3 + 1627200 * r_2 + 14364000 * r_1 - 58713721}{1209600.}$$

$$q_{44} = 0$$

$$q_{45} = -\frac{9450000 * r_3 + 200635200 * r_2 + 1747116000. * r_1 - 7263657599.}{3.26592e7}$$

$$q_{46} = \frac{604800 * r_3 + 13363200 * r_2 + 120960000 * r_1 - 485920643}{3.26592e7}$$

$$q_{55} = 0$$

$$q_{56} = \frac{415800 * r_3 + 8604000 * r_2 + 72954000 * r_1 - 286439017}{3.26592e7}$$

$$q_{66} = 0$$

D.3. Eight order accurate operators

We now present the specific form of the eighth order accurate operators used in the analysis. The discrete norm H at the boundary is defined as

$h_{1,1} = .17278828151304213131$	$h_{3,6} = -.86170509476217520096$
$h_{1,2} = .26442559491473446335$	$h_{3,7} = .23272822377785868580$
$h_{1,3} = -.31178196884312775720$	$h_{3,8} = -.27718561649605047808e - 1$
$h_{1,4} = .30943600415290628943$	$h_{4,4} = 4.5048009713827725943$
$h_{1,5} = -.22687886379977231568$	$h_{4,5} = -2.8194294132418145464$
$h_{1,6} = .10699051704359999240$	$h_{4,6} = 1.4139447698567646313$
$h_{1,7} = -.29198436836537438395e - 1$	$h_{4,7} = -.40168231609234325290$
$h_{1,8} = .35313167405158916567e - 2$	$h_{4,8} = .49803339945923016666e - 1$
$h_{2,2} = 1.7526198409167495775$	$h_{5,5} = 3.3650057528838514157$
$h_{2,3} = -1.1935018761521814908$	$h_{5,6} = -1.2261739857055893831$
$h_{2,4} = 1.3954360831111377900$	$h_{5,7} = .35734819363435995274$
$h_{2,5} = -1.0175504328863858993$	$h_{5,8} = -.45187886555639925953e - 1$
$h_{2,6} = .47894397921583602822$	$h_{6,6} = 1.6529897067349637657$
$h_{2,7} = -.13175544973723205885$	$h_{6,7} = -.19435314011455700920$
$h_{2,8} = .16150503562667126340e - 1$	$h_{6,8} = .24990727889886053755e - 1$
$h_{3,3} = 2.9309103416555983901$	$h_{7,7} = 1.0588289336073241051$
$h_{3,4} = -2.4589576423781345782$	$h_{7,8} = -.76680474804950146879e - 2$
$h_{3,5} = 1.8303365981930377633$	$h_{8,8} = 1.0010106996984233357$

The discrete difference operator approximating $\frac{d}{dx}$ we denote (here) $D_1 = H^{-1}Q$, obeying our wanted SBP property

$D1_{1,1} = -2.592857142857143d0$	$D1_{3,9} = -0.0010055472165286575d0$	$D1_{6,5} = -1.1039047461210942d0$
$D1_{1,2} = 7.0d0$	$D1_{3,10} = 3.8794759110886745d - 4$	$D1_{6,6} = 0.27359438161151506d0$
$D1_{1,3} = -10.500000000000002d0$	$D1_{3,11} = -6.8704635776930775d - 5$	$D1_{6,7} = 0.63460627616441168d0$
$D1_{1,4} = 11.66666666666667d0$	$D1_{3,12} = 5.0082327516880903d - 6$	$D1_{6,8} = -0.1334700237623892d0$
$D1_{1,5} = -8.750000000000053d0$	$D1_{4,1} = -0.01374973021859196d0$	$D1_{6,9} = 0.020553664597517285d0$
$D1_{1,6} = 4.200000000000064d0$	$D1_{4,2} = 0.13486302290702401d0$	$D1_{6,10} = -5.2448374888321939d - 4$
$D1_{1,7} = -1.1666666666666703d0$	$D1_{4,3} = -0.72696910885431376d0$	$D1_{6,11} = -3.5364415168681655d - 4$
$D1_{1,8} = 0.14285714285714438d0$	$D1_{4,4} = 0.017812686448076227d0$	$D1_{6,12} = 1.9848170711942382d - 5$
$D1_{1,9} = 0.$	$D1_{4,5} = 0.6393775076060112d0$	$D1_{7,1} = 0.0012022691922812573d0$
$D1_{1,10} = 0.$	$D1_{4,6} = 0.022147920488592564d0$	$D1_{7,2} = -0.0099404639226380095d0$
$D1_{1,11} = 0.$	$D1_{4,7} = -0.12565765302041595d0$	$D1_{7,3} = 0.039882284654387555d0$
$D1_{1,12} = 0.$	$D1_{4,8} = 0.068585850834641665d0$	$D1_{7,4} = -0.11500484724090931d0$
$D1_{2,1} = -0.14298292410192714d0$	$D1_{4,9} = -0.019233942555101392d0$	$D1_{7,5} = 0.30419289144259271d0$
$D1_{2,2} = -1.4489927866116712d0$	$D1_{4,10} = 0.0031486152221289702d0$	$D1_{7,6} = -0.89394403806786826d0$
$D1_{2,3} = 2.9964729239178829d0$	$D1_{4,11} = -3.4332575058906574d - 4$	$D1_{7,7} = 0.056932295488355524d0$
$D1_{2,4} = -2.4929493873234359d0$	$D1_{4,12} = 1.8156892537446339d - 5$	$D1_{7,8} = 0.77700125713081891d0$
$D1_{2,5} = 1.6578787083897146d0$	$D1_{5,1} = 0.0088862667686782706d0$	$D1_{7,9} = -0.19389096736102715d0$
$D1_{2,6} = -0.7430309325660327d0$	$D1_{5,2} = -0.081997207069678529d0$	$D1_{7,10} = 0.037021801268937171d0$
$D1_{2,7} = 0.19660315690279093d0$	$D1_{5,3} = 0.36016066918405126d0$	$D1_{7,11} = -0.0034453239617136533d0$
$D1_{2,8} = -0.022921081922677878d0$	$D1_{5,4} = -1.138622537383166d0$	$D1_{7,12} = -7.1586232168436659d - 6$
$D1_{2,9} = -5.9765761149596457d - 5$	$D1_{5,5} = 0.45753588027993108d0$	$D1_{8,1} = -1.7018888206312392d - 4$

$D1_{2,10} = -2.086075830489387d - 5$	$D1_{5,6} = 0.38914191081194799d0$	$D1_{8,2} = 0.001407457714362741d0$
$D1_{2,11} = 3.0132094578465812d - 6$	$D1_{5,7} = 0.047353759946214852d0$	$D1_{8,3} = -0.0051428241139400005d0$
$D1_{2,12} = -6.3374647316878056d - 8$	$D1_{5,8} = -0.060707854441402261d0$	$D1_{8,4} = 0.014469260937249902d0$
$D1_{3,1} = 0.024035178364099158d0$	$D1_{5,9} = 0.022163172460071972d0$	$D1_{8,5} = -0.052868823562666749d0$
$D1_{3,2} = -0.33511996288598189d0$	$D1_{5,10} = -0.004385536290694581d0$	$D1_{8,6} = 0.21333416109695102d0$
$D1_{3,3} = -0.77719249965062054d0$	$D1_{5,11} = 4.9895905469285538d - 4$	$D1_{8,7} = -0.80809452640150636d0$
$D1_{3,4} = 1.6547851227840236d0$	$D1_{5,12} = -2.7483320646974942d - 5$	$D1_{8,8} = 0.0032794907268712007d0$
$D1_{3,5} = -0.81942145154188328d0$	$D1_{6,1} = -0.0035154238926503028d0$	$D1_{8,9} = 0.79912442343041246d0$
$D1_{3,6} = 0.32374316200170666d0$	$D1_{6,2} = 0.032627145467311741d0$	$D1_{8,10} = -0.19984491904967425d0$
$D1_{3,7} = -0.080342166504192805d0$	$D1_{6,3} = -0.1441805719128838d0$	$D1_{8,11} = 0.038076865351646491d0$
$D1_{3,8} = 0.010193913461294177d0$	$D1_{6,4} = 0.42454757757811995d0$	$D1_{8,12} = -0.0035703772476434379d0$

In the interior we have the eighth order accurate central operator

$$h(D_1 v)_j = \frac{1}{280} v_{j-4} - \frac{4}{105} v_{j-3} + \frac{1}{5} v_{j-2} - \frac{4}{5} v_{j-1} + \frac{4}{5} v_{j+1} - \frac{1}{5} v_{j+2} + \frac{4}{105} v_{j+3} - \frac{1}{280} v_{j+4}.$$

The discrete difference operator approximating $\frac{d^2}{dx^2}$ obeying our wanted SBP property is written $D_2 = H^{-1}(-A + BS)$, where $A + A^T \geq 0$. The interior stencil is the standard eight order accurate central scheme

$$h^2(D_2 v)_j = -\frac{1}{560} v_{j-4} + \frac{8}{315} v_{j-3} - \frac{1}{5} v_{j-2} + \frac{8}{5} v_{j-1} - \frac{205}{72} v_j + \frac{8}{5} v_{j+1} - \frac{1}{5} v_{j+2} + \frac{8}{315} v_{j+3} - \frac{1}{560} v_{j+4}.$$

At the boundary the operator with a sixth order boundary closure becomes

$D2(1, 1) = 0.459559486573298D1$	$D2(3, 9) = -0.3982789723630851D - 1$	$D2(6, 5) = 0.9837460406594241D0$
$D2(1, 2) = -0.1737587003697495D2$	$D2(3, 10) = 0.3613749551360845D - 3$	$D2(6, 6) = -0.2324548401306039D1$
$D2(1, 3) = 0.2671554512941234D2$	$D2(3, 11) = -0.4325584278035533D - 4$	$D2(6, 7) = 0.1311841356539494D1$
$D2(1, 4) = -0.182533124810469D2$	$D2(3, 12) = 0.2504116375844045D - 5$	$D2(6, 8) = -0.1004519515199941D0$
$D2(1, 5) = -0.208613717646915D1$	$D2(4, 1) = 0.413834452956972D - 2$	$D2(6, 9) = 0.5233628499353206D - 2$
$D2(1, 6) = 0.1436890974117532D2$	$D2(4, 2) = -0.9317382863354466D - 1$	$D2(6, 10) = 0.5458274935095434D - 3$
$D2(1, 7) = -0.1157334375947655D2$	$D2(4, 3) = 0.1296278911778636D1$	$D2(6, 11) = -0.2121077126646392D - 3$
$D2(1, 8) = 0.4224129963025046D1$	$D2(4, 4) = -0.2301454617412467D1$	$D2(6, 12) = 0.9924085355971193D - 5$
$D2(1, 9) = -0.6155162453781307D0$	$D2(4, 5) = 0.9496907454250803D0$	$D2(7, 1) = 0.2798761681044611D - 2$
$D2(1, 10) = 0.D0$	$D2(4, 6) = 0.3211654316623705D0$	$D2(7, 2) = -0.2273831582632708D - 1$
$D2(1, 11) = 0.D0$	$D2(4, 7) = -0.2522929099188442D0$	$D2(7, 3) = 0.7941253606056085D - 1$
$D2(1, 12) = 0.D0$	$D2(4, 8) = 0.930043044984534D - 1$	$D2(7, 4) = -0.1414647886625625D0$
$D2(2, 1) = 0.7663483674837219D0$	$D2(4, 9) = -0.1951026759150047D - 1$	$D2(7, 5) = 0.1676244442372628D - 1$
$D2(2, 2) = -0.9196803752511684D0$	$D2(4, 10) = 0.2348749011339006D - 2$	$D2(7, 6) = 0.1416153480495742D1$
$D2(2, 3) = -0.842207972743573D0$	$D2(4, 11) = -0.2039417953611042D - 3$	$D2(7, 7) = -0.2745855902808057D1$
$D2(2, 4) = 0.1034353161256694D1$	$D2(4, 12) = 0.9078446268723169D - 5$	$D2(7, 8) = 0.1564969049973078D1$
$D2(2, 5) = 0.9224566003381633D0$	$D2(5, 1) = 0.9702030996040648D - 2$	$D2(7, 9) = -0.192894978753717D0$
$D2(2, 6) = -0.1915904204050834D1$	$D2(5, 2) = -0.6794130076783107D - 1$	$D2(7, 10) = 0.2457122826770361D - 1$
$D2(2, 7) = 0.1358106271667133D1$	$D2(5, 3) = 0.1333345846555384D0$	$D2(7, 11) = -0.1709935539582438D - 2$
$D2(2, 8) = -0.4698818319034839D0$	$D2(5, 4) = 0.9149526892124103D0$	$D2(7, 12) = -0.3579311608421833D - 5$
$D2(2, 9) = 0.6642475553490265D - 1$	$D2(5, 5) = -0.1957269586741238D1$	$D2(8, 1) = -0.4040429839128132D - 3$
$D2(2, 10) = -0.163599150014082D - 4$	$D2(5, 6) = 0.8452193170274778D0$	$D2(8, 2) = 0.3282528546989832D - 2$
$D2(2, 11) = 0.1619270768597741D - 5$	$D2(5, 7) = 0.2160399635643034D0$	$D2(8, 3) = -0.117215310517751D - 1$
$D2(2, 12) = -0.3168732365843903D - 7$	$D2(5, 8) = -0.1182303495391327D0$	$D2(8, 4) = 0.2230119016828276D - 1$
$D2(3, 1) = -0.9930472508132245D - 1$	$D2(5, 9) = 0.2723622874009121D - 1$	$D2(8, 5) = -0.589253331879865D - 2$
$D2(3, 2) = 0.1494543277053003D1$	$D2(5, 10) = -0.3328174251388732D - 2$	$D2(8, 6) = -0.1734623416535851D0$
$D2(3, 3) = -0.317028822529708D1$	$D2(5, 11) = 0.2983387640521609D - 3$	$D2(8, 7) = 0.1585367510775726D1$
$D2(3, 4) = 0.2864206231232483D1$	$D2(5, 12) = -0.1374166032348747D - 4$	$D2(8, 8) = -0.2842164305683002D1$

$D2(3, 5) = -0.2207907708688962D1$	$D2(6, 1) = -0.7955850076892026D - 2$	$D2(8, 9) = 0.1598973239836509D1$
$D2(3, 6) = 0.1847596328819334D1$	$D2(6, 2) = 0.628530334801436D - 1$	$D2(8, 10) = -0.199880296017579D0$
$D2(3, 7) = -0.9882048151539512D0$	$D2(6, 3) = -0.2054352689917416D0$	$D2(8, 11) = 0.2538577000496714D - 1$
$D2(3, 8) = 0.298866911124072D0$	$D2(6, 4) = 0.2743737688500514D0$	$D2(8, 12) = -0.1785188623821719D - 2$

and with a seventh order boundary derivative operator

$$BS = \frac{1}{h} \begin{bmatrix} -ds_1 & -ds_2 & -ds_3 & -ds_4 & -ds_5 & -ds_6 & -ds_7 & -ds_8 & -ds_9 \\ & & & 0 & & & & & \\ & & & & \ddots & & & & \\ & & & & & 0 & & & \\ & ds_9 & ds_8 & ds_7 & ds_6 & ds_5 & ds_4 & ds_3 & ds_2 & ds_1 \end{bmatrix}$$

$$ds_1 = -\frac{26605318914871}{10574000000000} \qquad ds_5 = -\frac{7142764970579}{2114800000000}$$

$$ds_2 = \frac{16881394988747}{2643500000000} \qquad ds_6 = -\frac{259035026131}{2643500000000}$$

$$ds_3 = -\frac{44151764954129}{5287000000000} \qquad ds_7 = \frac{5193568357271}{5287000000000}$$

$$ds_4 = \frac{19479098298429}{2643500000000} \qquad ds_8 = -\frac{1245462146053}{2643500000000}$$

$$ds_9 = \frac{76749811}{1000000000}$$

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