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High-Order Compact-Stencil Summation-By-Parts Operators for the Second Derivative with Variable Coefficients

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Abstract: A general framework is presented for deriving compact-stencil high-order summation-by-parts (SBP) finite-difference operators for the second derivative with variable coefficients with 4^{th} through 6^{th} order accuracy. These second-derivative operators are compatible with the first derivative SBP operator, possess the same norm, and can therefore be used to construct time stable numerical schemes with simultaneous approximation terms to weakly impose boundary conditions. The derivation of these operators leads to various free parameters which can be used for optimization of the operator about criteria such as spectral radius and truncation error. Numerical tests on the one-dimensional linear convection-diffusion equation using the method of manufactured solutions are used for verification and characterization studies, demonstrating that the compact operators have lower global error and better accuracy than application of the first derivative twice.

Keywords: Summation by parts, compact stencil, finite difference, higher-order methods.

1 Introduction

Since the seminal work of Kreiss and Oliger [1] and Swartz and Wendroff [2], the computational efficiency of higher-order (HO) methods has been recognized. In the asymptotic region, the local truncation error of HO methods is of order $O(\Delta x)^p$, where $p \geq 3$, and Δx is the mesh spacing. Thus, for a given accuracy, HO methods require coarser mesh spacing relative to lower-order methods. HO methods have been shown to be more computationally efficient than lower-order methods; some examples are the linear advection equation [3] and the compressible Navier-Stokes (NS) equations [4, 5]. Here the HO discretization employed is a combination of summation-by-parts (SBP) finite-difference operators, [6, 7, 8, 9, 8, 10, 11, 12] with simultaneous approximation terms (SATs) for boundary and interface treatment [13, 14, 15, 16, 17, 18, 19, 20, 21, 22], which have been successfully applied to various problems including, the linear advection diffusion equation [23], electromagnetic wave propagation [24], and the compressible Euler and NS equations [17, 19, 22].

The main difficulty in implementing HO methods arises from the boundary treatment. SBP operators provide a systematic means of deriving HO finite-difference operators with suitably HO boundary treatment that are time-stable [11]. In conjunction with SATs to weakly impose boundary conditions, SBP operators naturally give rise to multi-block schemes that have low communication overhead, which is advantageous for parallel computations. This results from the fact that only C^0 continuity needs to be maintained between blocks and, regardless of the order of the scheme, the same amount of information is passed between blocks, i.e. there is no need for halo nodes. In curvilinear coordinates, time stability can only be proven for diagonal-norm SBP operators [25]; thus we limit ourselves to those operators. The disadvantage of diagonal-norm SBP operators is that while the interior scheme is $2p$ accurate, the boundary treatment is p order accurate and the global order of accuracy is $p+1$ [26]. However, Mattsson and Nordström [8] have shown that if the PDE contains a second derivative, utilization of the compact-stencil SBP formulation for the second derivative garners an additional degree of accuracy, and so the method is formally $p+2$ order accurate. Finally, Hicken and Zingg [27] have shown that if the formulation is dual consistent, then functionals converge with the order of accuracy of the interior scheme.

Compact-stencil operators have been shown to have various numerical advantages over non-compact-stencil operators (application of the first derivative twice) [11]: they have lower global error, and are more dissipative of high wavenumber modes. Moreover, they have a smaller bandwidth and thus require less computational resources, particularly if one is interested in adjoint-based optimization for which the Jacobian must be constructed. Finally, although one can use the application of the first-derivative twice, doing so with SBP operators results in the loss of one additional order of accuracy.

The present paper is concerned with presenting a general framework for derivation of higher-order maximally-compact-stencil SBP operators for the second derivative with variable coefficients. Recent work by Mattsson [12] presents maximally-compact-stencil SBP operators up to 5^{th} order accuracy. Here we will present a new derivation for maximally-compact-stencil operators that generalizes to higher order, with better accuracy characteristics, and reduces the number of equations that need to be solved. These operators are validated using the one-dimensional linear convection-diffusion equation.

2 Spatial Discretization

Here we introduce summation by parts (SBP) finite-difference operators for the first derivative, the second derivative with constant coefficients, and the second derivative with variable coefficients. The SBP operators for the first derivative were first derived by Kreiss and Scherer [6], refined by Strand [7], and applied by various authors (see [11],[28], [9], [29]). SBP operators are centred difference schemes that do not include boundary conditions; these must be taken care of by some other means, in our case using SATs, see Section 3. Ultimately we are interested in the solution of the compressible NS equations over complex geometries. In order to capture these geometries we use structured meshes, so we transform the NS equations to curvilinear coordinates. As a result, we limit the discussion of SBP operators to those with a diagonal-norm, as these are the only SBP operators that can be proven to be time-stable in curvilinear coordinates [25] . Given our interest in the NS equations, the goal is to construct a finite-difference approximation to $\partial_x(\beta\partial_x Q)$ that is conservative, has the SBP property, and is compatible with the first derivative such that it can be used to prove time stability for the linearized NS equations [11]. In line with our goal to garner interest in the SBP SAT approach, we present detailed derivations of the required derivatives that are 4^{th}-order in the interior of the domain as examples.

2.1 Notation and definitions

We follow the conventions laid out by Hicken and Zingg [30]. SBP difference operators are generically defined on a uniformly spaced grid of $N+1$ points on the domain $[0,1]$ and thus the grid spacing is $\Delta x = 1/N$. Typically the domain we are interested in is not $[0,1]$, but we assume that for the set of problems of interest a sufficiently differentiable invertible transformation exists from the domain of interest to $[0,1]$.

Capital letters with a script type are used to denote functions on a specified domain, and so $\mathcal{U}(x) \in C^p[a,b]$ denotes that the function, $\mathcal{U}(x)$, is a p times differentiable function on $[a,b]$. Roman letters in bold font denote the restriction $\mathcal{U}(x)$ onto a $N+1$ grid of corresponding continuous functions, as an example $\mathbf{u} \in \mathbb{R}^{N+1}$ means $\mathbf{u} = [\mathcal{U}(x_0), \mathcal{U}(x_1), .., \mathcal{U}(x_N)]^T$. In discussing the imposition of boundary conditions using SATs, we refer to the unit vectors $\mathbf{e}_L, \mathbf{e}_R \in \mathbb{R}^{N+1}$, which are

$$\mathbf{e}_L = [1, 0, ..., 0]^T, \mathbf{e}_R = [0, .., 0, 1]^T.$$

The operators for the first and second derivatives have different orders of accuracy on the interior, at the boundary, and globally. In order to differentiate between operators and the various orders of accuracy we follow the convention that we append a superscript to operators for the various orders of accuracy and a subscript to denote which derivative we are approximating, for example, $D_{i,e}^{(a,b,c)}$, denotes the operator for the i^{th} derivative with interior order of accuracy of a, boundary closure accuracy of b and results in a solution with global order of accuracy c, while the additional subscript e is to differentiate amongst various versions of the operator. In some cases we will not be interested in one or several of the orders of accuracy and will insert colons; as an example; $D_3^{(2,:,:)}$ denotes a second-order approximation to the third derivative where we specify neither the accuracy of the operator at the boundary nor the global order of accuracy. For the second derivative with variable coefficients we will make explicit the dependence on the variable coefficients, β, by denoting these operators as $D_2^{(a,b,c)}(B)$, where B is a diagonal matrix with the variable coefficients along its diagonal.

2.2 First derivative

For the first derivative, the SBP property is mimetic of $\int_a^b \mathcal{Q}\partial_x \mathcal{Q} dx$, which leads to the following definition:

SBP Diagonal Norm First Derivative The matrix $D \in R^{(N+1)\times(N+1)}$ is an SBP operator for the first derivative if it approximates the first derivative and is of the form $D = H^{-1}\Theta$, where $H \in R^{(N+1)\times(N+1)}$, is a positive-definite diagonal matrix, called the norm, and Θ has property $\Theta + \Theta^T = \mathrm{diag}(-1, 0, ..., 0, 1)$.

To understand the SBP property, first let us define the inner product of two real valued-functions, $\mathcal{U}, \mathcal{V} \in [0, 1]$ by $(\mathcal{U}, \mathcal{V}) = \int_0^1 \mathcal{U}\mathcal{V} dx$, and hence the norm $||\mathcal{U}|| = \sqrt{\int_0^1 \mathcal{U}^2 dx}$. Now consider the linear convection equation,

$$\frac{\partial \mathcal{Q}}{\partial t} = -\frac{\partial \mathcal{Q}}{\partial x}. \tag{1}$$

The energy method involves multiplying (1) by $\mathcal{Q}$ and integrating in space, i.e. taking the inner product of the PDE with respect to the solution $\mathcal{Q}$. We get

$$\frac{d||\mathcal{Q}||^2}{dt} = -\left. \mathcal{Q}^2 \right|_0^1, \tag{2}$$

and we can see that stability of the equations depends solely on the boundary values of $\mathcal{Q}$. The semi-discrete form of the linear convection equation is

$$\frac{dq}{dt} = -D\mathbf{q} = -H^{-1}\Theta\mathbf{q}. \tag{3}$$

We similarly define a discrete inner product and norm as $(\mathbf{u}, \mathbf{v})_H = \mathbf{u}^T H \mathbf{v}$ and $||\mathbf{u}||_H = \sqrt{\mathbf{u}^T H \mathbf{u}}$. Taking the discrete inner product of (3), i.e. multiplying through by $\mathbf{q}^T H$, and adding the transpose, based on the properties of H and Θ, gives

$$\frac{d||\mathbf{q}||_H^2}{dt} = -\left. \mathbf{q}^2 \right|_0^1,$$

and we can see that the SBP property is mimetic, in the discrete case, of integration by parts and thus the energy method. SBP operators for the first derivative have been well studied (see [7], [9], [21], [14], [16], [18], [31], [32]). Here we present a brief account of how to derive them. We are interested in compact-stencil centred-difference approximations of the first derivative that satisfy the SBP property. Various definitions of compact-stencil exist; here we mean operators that in the interior have the same number of nodes as the compact first-derivative operator in the interior, i.e. $2p + 1$ nodes. The interior stencil is known, so we need only concentrate on deriving the stencil at boundary points. To summarize what we know about $D = H^{-1}\Theta$:

1. D is $2p$ accurate at interior points and p accurate at $2p$ points at the left and right boundaries [7];
2. $\Theta^T + \Theta = \mathrm{diag}(-1, 0, 0, ..., 0, 0, 1)$ implying that Θ is nearly skew-symmetric with $\Theta(1, 1) = -\frac{1}{2}$, $\Theta(N + 1, N + 1) = \frac{1}{2}$, and the remaining diagonal entries are 0;
3. H is diagonal and positive definite.

We use $D_1^{(4,2,3)}$ as an example, i.e. $p = 2$. Since it is 4^{th} order in the interior, this means that we have a 5-point interior stencil, and we have 4 boundary stencils that need to be derived. The global order of accuracy of the solution is $p+1=3$. The interior stencil is given as $(\frac{1}{12}, -\frac{2}{3}, 0, \frac{2}{3}, -\frac{1}{12},)$, so we have that

$$D=H^{-1}\Theta=\begin{bmatrix} \frac{1}{H_{1,1}} & & & & & \\ & \frac{1}{H_{2,2}} & & & & \\ & & \frac{1}{H_{3,3}} & & & \\ & & & \frac{1}{H_{4,4}} & & \\ & & & & 1 & \\ & & & & & \ddots \end{bmatrix} \times \begin{bmatrix} -\frac{1}{2} & \theta_{1,2} & \theta_{1,3} & \theta_{1,4} & & & & & \\ -\theta_{1,2} & 0 & \theta_{2,3} & \theta_{2,4} & & & & & \\ -\theta_{1,3} & -\theta_{2,3} & 0 & \theta_{3,4} & \frac{1}{12} & & & & \\ -\theta_{1,4} & -\theta_{2,4} & -\theta_{3,4} & 0 & \frac{2}{3} & -\frac{1}{12} & & & \\ 0 & 0 & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & & \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots & \end{bmatrix}.$$

Note that the above form is based upon the minimum boundary stencil width, as derived by Strand [7], to satisfy order $2p$ accuracy on the interior and order p accuracy at $2p$ points. The $D_1^{(4,2,3)}$ operator gives the following approximations at the boundary nodes

$$\text{Node 1: } \frac{1}{H_{1,1}}\left(-\tfrac{1}{2}q_j + \theta_{1,2}q_{j+1} + \theta_{1,3}q_{j+2} + \theta_{1,4}q_{j+3}\right),$$

$$\text{Node 2: } \frac{1}{H_{2,2}}\left(-\theta_{1,2}q_{j-1} + \theta_{2,3}q_{j+1} + \theta_{2,4}q_{j+2}\right)$$

$$\vdots$$

The above equations must satisfy our accuracy criteria, in this case second-order accuracy. Inserting Taylor series expansions of the q_js, we get a system of equations; as an example from the first node we have

$$-\tfrac{1}{2} + \theta_{1,2} + \theta_{1,3} + \theta_{1,4} = 0,$$

$$\theta_{1,2} + 2\,\theta_{1,3} + 3\,\theta_{1,4} = H_{1,1},$$

$$\tfrac{1}{2}\,\theta_{1,2} + 2\,\theta_{1,3} + \tfrac{9}{2}\,\theta_{1,4} = 0.$$

The reader will note that there are $\frac{2p(2p-1)}{2} = 6$ coefficients but there are $2p(p+1) = 12$ equations, and so the system appears overdetermined. However, this does not turn out to be the case since not all of the equations are linearly independent. In fact, the following occurs: for $D_1^{(2,1,2)}$ and $D_1^{(4,2,3)}$, the operators are unique, while for $D_1^{(6,3,4)}$ and $D_1^{(8,4,5)}$, the operators have 1 and 3 free parameters respectively that can be used to optimize their behaviour. For interior orders beyond 8, no solutions can be found with H being positive definite and hence a discrete norm, see [7]. In order to surpass these limitations one could increase the interior stencil width, see [9]. The operators $D_1^{(2,1,2)}$, $D_1^{(6,3,4)}$ and $D_1^{(8,4,5)}$ are given in Appendix A.

2.3 Second derivative

The discrete SBP operator for the second derivative with variable coefficients results in a large system of non-linear equations that must be solved for the boundary closures. As the order of the operator increases so too does the complexity of the system of non-linear equations that needs to be solved and the number of free parameters that need to be specified once a solution is found. The second derivative with constant coefficients is a specific instance of the second derivative with variable coefficients and therefore the second derivative with variable coefficients must collapse onto it. We derive the second derivative with constant coefficients to use it as a means of restricting the solution space of the second derivative with variable coefficients.

First we define the SBP operators for the second derivative with constant and variable coefficients, give a generic structure to construct them, and then deal with each in subsections. We define the discrete SBP operator for the second derivative with constant coefficients, $B = \mathrm{diag}(1, \ldots, 1)$, and variable coefficients as follows:

SBP Second Derivative The matrix $D_2^{(2p,p,p+2)}(B) \in R^{(N+1)\times(N+1)}$ is an SBP operator for the second derivative if it approximates the second derivative and is of the form, $D_2^{(2p,p,p+2)}(B) = H^{-1}\{-M + EBD_b\}$, where H is a diagonal positive-definite matrix called the norm, $E = \mathrm{Diag}(-1, 0, ..., 0, 1)$, $B = \mathrm{diag}(\beta_0, \ldots, \beta_N)$,

$D_b^{(:,p+1,:)}$ is an approximation to the first derivative at the boundaries, $M = \left(D_1^{(2p,p,p+1)}\right)^T HBD_1^{(2p,p,p+1)} + R$, M, and R are positive-semi-definite (PSD) and symmetric, and B is PSD.

In order to show that the proposed SBP-SAT discretization is time-stable for the linearized NS equations, H in the above definition must be the same norm as used with the first derivative. Thus the formulation is said to be compatible with the first derivative; see Mattsson [10].

To construct these operators, we need R. For the $p+2$ globally accurate operator, we posit the general form:

$$R_{p+2} = \frac{1}{h}\sum_{i=p+1}^{2p} \alpha_i (\tilde{D}_{i,p+2}^{(2,1,:)})^T C_i^{(p+2)} B \tilde{D}_{i,p+2}^{(2,1,:)},$$

where h is the mesh spacing. For the construction of R, $\tilde{D}_i^{(2,1,:)}$ has the same number of entries as the compact-stencil first derivative in the interior. The tilde notation denotes an undivided difference approximation. Constructed thus, the operator is guaranteed to be PSD, as long as the C_i, which are diagonal matrices of the form $C_i^{(p+2)} = \text{diag}\left(c_{11}^{(p+2)}, \ldots, c_{2p2p}^{(p+2)}, 1, \ldots, 1, c_{2p2p}^{(p+2)}, \ldots, c_{11}^{(p+2)}\right)$, where the superscript $(p+2)$ is to differentiate amongst the various C_i, are PSD.

The interior stencil that is compatible with the proposed construction of the second derivative is given as

$$D_{2,\text{int}}^{(2p,:,:)} = -\left\{(D^{(2p,:,:)})^T B D^{(2p,:,:)} + \frac{1}{h^2}\sum_{p+1}^{2p} \alpha_i (\tilde{D}_{i,p+2}^{(2,:,:)})^T B \tilde{D}_{i,p+2}^{(2,:,:)}\right\}.$$

We are limited to 8^{th}-order interior accuracy if we want to retain the compact stencil, so we can explicitly give the general form of the SBP operators for orders $2, 4, 5$, and 6 as

$$\begin{aligned}
D_2^{(2,1,2)}(B) &= H^{-1}\left\{-\left(D_1^{(2,1,2)}\right)^T HBD_1^{(2,1,2)} - \tfrac{1}{4h}\left(\tilde{D}_2^{(2,1,:)}\right)^T C_2^{(2)} B\tilde{D}_2^{(2,1,:)} + \tfrac{1}{h} EB\tilde{D}_1^{(:,2,:)}\right\}, \\
D_2^{(4,2,4)}(B) &= H^{-1}\left\{-\left(D_1^{(4,2,3)}\right)^T HBD_1^{(4,2,3)} - \tfrac{1}{18h}\left(\tilde{D}_3^{(2,1,:)}\right)^T C_3^{(4)} B\tilde{D}_3^{(2,1,:)}\right. \\
&\qquad \left. -\tfrac{1}{48h}\left(\tilde{D}_{4,4}^{(2,1,:)}\right)^T C_4^{(4)} B\tilde{D}_{4,4}^{(2,1,:)} + \tfrac{1}{h} EB\tilde{D}_1^{(:,3,:)}\right\}, \\
D_2^{(6,3,5)}(B) &= H^{-1}\left\{-\left(D_1^{(6,3,4)}\right)^T HBD_1^{(6,3,4)} - \tfrac{1}{80h}\left(\tilde{D}_{4,5}^{(2,1,:)}\right)^T C_4^{(5)} B\tilde{D}_{4,5}^{(2,1,:)}\right. \\
&\qquad \left. - \tfrac{1}{100h}\left(\tilde{D}_{5,5}^{(2,1,:)}\right)^T C_5^{(5)} B\tilde{D}_{5,5}^{(2,1,:)} - \tfrac{1}{720h}\left(\tilde{D}_{6,6}^{(2,1,:)}\right)^T C_6^{(5)} B\tilde{D}_{6,6}^{(2,1,:)} + \tfrac{1}{h} EB\tilde{D}_1^{(:,4,:)}\right\}, \\
D_2^{(8,4,6)}(B) &= H^{-1}\left\{-\left(D_1^{(8,4,5)}\right)^T HBD_1^{(8,4,5)} - \tfrac{1}{350h}\left(\tilde{D}_{5,6}^{(2,1,:)}\right)^T C_5^{(6)} B\tilde{D}_{5,6}^{(2,1,:)}\right. \\
&\qquad -\tfrac{1}{252h}\left(\tilde{D}_{6,6}^{(2,1,:)}\right)^T C_6^{(6)} B\tilde{D}_{6,6}^{(2,1,:)} - \tfrac{1}{980h}\left(\tilde{D}_7^{(2,1,:)}\right)^T C_7^{(6)} B\tilde{D}_7^{(2,1,:)} \\
&\qquad \left. -\tfrac{1}{11200h}\left(\tilde{D}_8^{(2,1,:)}\right)^T C_8^{(6)} B\tilde{D}_8^{(2,1,:)} + \tfrac{1}{h} EB\tilde{D}_1^{(:,5,:)}\right\}.
\end{aligned} \tag{4}$$

Without additional restrictions, the above formulation leads to a very large system of highly nonlinear equations, which are difficult to solve and lead to a large number of free parameters. However, our experience with the first derivative and the second derivative with constant coefficients leads us to anticipate a certain degree of cancelation and a particular form of the operators. Specifically, we expect

- p^{th} order accuracy at $2p$ boundary nodes at the left and right boundary, with the remaining nodes having accuracy of $2p$; these will be called the accuracy constraints;

- M is symmetric and so we have a $2p \times 2p$ block of unknowns at each boundary; these will be called the form constraints.

These restrictions lead to operators that have preferable accuracy characteristics, more nodes that are $2p$ accurate, and smaller stencil size at boundary nodes. Moreover, our hope is that with these restrictions we should be able to simplify the process and reduce the number of free parameters.

2.4 SBP second derivative with constant coefficients

Operators with the SBP property for the second derivative with constant coefficients were first derived by Mattsson and Nordström [10] and refined by Mattsson et al. [11]; operators of accuracy $D_2^{(2,1,2)}$,$D_2^{(4,2,4)}$,$D_2^{(6,3,5)}$, and $D_2^{(8,4,6)}$ were derived in the latter. Mattsson and Nordström [10] proved that the second derivative can have boundary closures with order of accuracy of p but retain global order of accuracy $p+2$. However, the authors did not prove that for an arbitrary number of grid points their proposed $D_2^{(8,4,6)}$ operator leads to a time-stable scheme. We could use form (4); however we run into same problems as with the variable-coefficient case, namely solving a large system of non-linear equations. Instead we propose a second means that requires solution of a system of equations with fewer nonlinear terms but does not automatically satisfy the requirements for time stability, i.e. PSD M and R. In order to satisfy the PSD condition, we present a novel means of determining which members of the resultant operators are time stable for an arbitrary number of nodes.

First though, to understand the SBP property in the constant-coefficient case, consider the diffusion equation on the interval $[0, 1]$:

$$\frac{\partial \mathcal{Q}}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\partial \mathcal{Q}}{\partial x}\right). \tag{5}$$

Applying the energy method to (5) gives

$$\frac{d||\mathcal{Q}||^2}{dt} = 2\left(\mathcal{Q}\frac{\partial \mathcal{Q}}{\partial x}\right)\bigg|_0^1 - 2\int_0^1 \left(\frac{\partial \mathcal{Q}}{\partial x}\right)^2 dx. \tag{6}$$

The semi-discrete equations are

$$\frac{d\mathbf{q}}{dt} = H^{-1}\left\{-M + EBD_b\right\}\mathbf{q}.$$

Multiplying by $q^T H$ and adding the transpose of the product gives

$$\begin{aligned} \frac{d||\mathbf{q}||_H}{dt} &= 2\mathbf{q}^T ED_b\mathbf{q} - 2\mathbf{q}^T M\mathbf{q} \\ &= 2\mathbf{q}^T ED_b\mathbf{q} - 2(D\mathbf{q})^T HD\mathbf{q} - 2\mathbf{q}^T R\mathbf{q}, \end{aligned} \tag{7}$$

and we can see that (7) is mimetic of the continuous case (6) within the discretization error, i.e. the R term is of the same order as the discretization error. This is easiest to see by noting that $2\mathbf{q}^T ED_b\mathbf{q} = 2(q_N(D_b\mathbf{q})_N - q_0(D_b\mathbf{q})_0)$ and $2(D\mathbf{q})^T HD\mathbf{q}$ is the discrete approximation to $2\int_0^1 \left(\frac{\partial \mathcal{Q}}{\partial x}\right)^2 dx$. Also note that the PSD property of M and R is required to find an energy estimate.

As mentioned, we would like to avoid solving the large system of nonlinear equations that arises from (4) and propose a construction that leads to a system with fewer nonlinear terms. To understand how we do so, first we must explore the construction of the $\tilde{D}_i^{(2,1,:)}$ operators. These are constructed to mimic the pattern in the first-derivative operator. The operator $D_1^{(2p,p,p+1)}$ has $2p$ boundary nodes at either boundary that are p order accurate. By virtue of the fact that the Θ component of the operator is almost skew-symmetric, this means that the largest boundary stencil, in row $2p$, has $3p$ entries. Hence the operation $\left(D^{(2p,p,p+1)}\right)^T HD_1^{(2p,p,p+1)}$, leads to an operator that has $3p$ nodes at either boundary that do not have the interior stencil. Our construction of the $\tilde{D}_i^{(2,1,:)}$ mimics the first derivative; thus we implement $2p$

boundary nodes that are first-order approximations to the i^{th} derivative that have $3p$ entries. The operation $\left(\tilde{D}_i^{(2,1,:)}\right)^T C_i^{p+1} \tilde{D}_i^{(2,1,:)}$ results in a symmetric operator that has $3p \times 3p$ blocks of non-linear coefficients that need to be determined to give an operator that is p^{th}-order accurate at the boundary, the remaining entries coming from the interior stencil and they symmetry of the operator. We can replace these non-linear coefficients with new variables, taking advantage of the symmetry of the operator. As an example consider the $\left(\tilde{D}_3^{(2,1,:)}\right)^T C_3^{(4)} \tilde{D}_3^{(2,1,:)}$ component of the operator $D_2^{(4,2,4)}$: The interior stencil of $\left(\tilde{D}_3^{(2,1,:)}\right)^T C_3^{(4)} \tilde{D}_3^{(4,2,4)}$, has the form $(-\frac{1}{2}, 1, 0, -1, \frac{1}{2})$. Application of this operator twice leads to $(-\frac{1}{4}, 1, -1, -1, \frac{5}{2}, -1, -1, 1, -\frac{1}{4})$, and so we replace $\left(\tilde{D}_3^{(2,1,:)}\right)^T C_3^{(4)} \tilde{D}_3^{(2,1,:)}$, with $R_3^{(4)}$, which has form

$$R_3^{(4)} = \begin{bmatrix}
R3_{11} & R3_{12} & R3_{13} & R3_{14} & R3_{15} & R3_{16} & & & & & & & \\
R3_{12} & R3_{22} & R3_{23} & R3_{24} & R3_{25} & R3_{26} & & & & & & & \\
R3_{13} & R3_{23} & R3_{33} & R3_{34} & R3_{35} & R3_{36} & -\frac{1}{4} & & & & & & \\
R3_{14} & R3_{24} & R3_{34} & R3_{44} & R3_{45} & R3_{46} & 1 & -\frac{1}{4} & & & & & \\
R3_{15} & R3_{25} & R3_{35} & R3_{35} & R3_{55} & R3_{56} & -1 & 1 & -\frac{1}{4} & & & & \\
R3_{16} & R3_{26} & R3_{36} & R3_{36} & R3_{56} & R3_{66} & -1 & -1 & 1 & -\frac{1}{4} & & & \\
 & & -\frac{1}{4} & 1 & -1 & -1 & \frac{5}{2} & -1 & -1 & 1 & -\frac{1}{4} & & \\
 & & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\
 & & & & -\frac{1}{4} & 1 & -1 & -1 & \frac{5}{2} & -1 & -1 & 1 & -\frac{1}{4}
\end{bmatrix},$$

with the lower portion given as the permutation of the columns and rows of the upper portion. The new set of equations has substantially fewer nonlinearities, the nonlinearities in the $D_2^{(6,3,4)}$ and $D_2^{(8,4,6)}$ operators coming from the application of the first derivative twice. However, we no longer have a guarantee that M of the resultant operator is PSD, and we must determine a means of finding which members of the resultant family of operators satisfy this requirement.

To determine the PSD conditions on M, we break it up into three matrices, two boundary matrices for the left and right boundary and one for the interior nodes. For example consider the M matrix for the operator $D_2^{(4,2,4)}$:

$$M = M_L + M_{\text{int}} + M_R$$

where

$$M = \begin{bmatrix}
M_{11} & M_{12} & M_{13} & M_{14} & & & & & & & \\
M_{12} & M_{22} & M_{23} & M_{24} & & & & & & & \\
M_{13} & M_{23} & M_{33} & M_{34} & \frac{1}{12} & & & & & & \\
M_{14} & M_{24} & M_{34} & M_{44} & -\frac{4}{3} & \frac{1}{12} & & & & & \\
 & & \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & & & & \\
 & & & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\
 & & & & \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & & \\
 & & & & & \frac{1}{12} & -\frac{4}{3} & M_{44} & M_{34} & M_{24} & M_{14} \\
 & & & & & & \frac{1}{12} & M_{44} & M_{34} & M_{24} & M_{14} \\
 & & & & & & & M_{34} & M_{33} & M_{23} & M_{13} \\
 & & & & & & & M_{24} & M_{23} & M_{24} & M_{12} \\
 & & & & & & & M_{41} & M_{31} & M_{21} & M_{11}
\end{bmatrix}, M_L = \begin{bmatrix}
M_{11} & M_{12} & M_{13} & M_{14} & & & \\
M_{12} & M_{22} & M_{23} & M_{24} & & & \\
M_{13} & M_{23} & M_{33} & M_{34} & \frac{1}{12} & & \\
M_{14} & M_{24} & M_{34} & M_{44} & -\frac{4}{3} & \frac{1}{12} & \\
0 & 0 & 0 & 0 & 0 & 0 & \\
 & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots
\end{bmatrix},$$

$$
M_{\text{int}} = \begin{bmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots & & & & & & \\
& 0 & 0 & 0 & 0 & 0 & & & & & \\
& & \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & & & & \\
& & & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\
& & & & \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & & \\
& & & & & 0 & 0 & 0 & 0 & 0 & \\
& & & & & & \ddots & \ddots & \ddots & \ddots & \ddots
\end{bmatrix}, M_R = \begin{bmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots & & & \\
& 0 & 0 & 0 & 0 & 0 & & \\
& & \frac{1}{12} & -\frac{4}{3} & M_{44} & M_{34} & M_{24} & M_{14} \\
& & & \frac{1}{12} & M_{44} & M_{34} & M_{24} & M_{14} \\
& & & & M_{34} & M_{33} & M_{23} & M_{13} \\
& & & & M_{24} & M_{23} & M_{24} & M_{12} \\
& & & & M_{41} & M_{31} & M_{21} & M_{11}
\end{bmatrix}.
$$

Now M is PSD if M_L and M_{int} are PSD, since the sum of matrices that are PSD is PSD, and if M_L is PSD, then M_R is PSD. The interior stencil for centred-difference approximations to the second derivative leads to M_{int} being PSD; see Kamakoti and Pantano [33] for the proof of the variable-coefficient case, which assures us that the constant-coefficient case has the same property. Left then is M_L, which reduces to the requirement that the upper 4×4 matrix be PSD. Thus, in general, we have converted the conditions for M being PSD for an arbitrarily sized M, within the confines of the minimum number of nodes required for construction of the operator, to the conditions under which a $2p \times 2p$ matrix is PSD.

Still the question is not simple since the size of the $2p \times 2p$ matrix increases with the order of the operator. Here we present three alternative means of determining the PSD property ordered from most to least complex. Since the $2p \times 2p$ matrix we are interested in is symmetric and must be PSD, we can construct a Cholesky decomposition. However, aside from being difficult to do, this approach is made more difficult by the need to consider degenerate cases. Alternatively, we can construct the characteristic polynomial of the matrix and note that the coefficients of the polynomial must have alternating sign – see Horn [34]. Finally, we can do a numerical parameter search, optimizing the operator with respect to some criterion, and see which members satisfy the PSD property by doing an eigenvalue analysis. The resultant operators are presented in Appendix B, and we give optimized values for the free parameters that result in an M that is PSD. The optimization was conducted by taking the derivative of a known test function and minimizing the L_2 norm.

2.5 Second derivative with variable coefficients

Previous work [35] demonstrates the existence of SBP operators for the second derivative that are more compact than the application of the first derivative twice. The work by Kamakoti et al. [33] proved the existence of maximally-compact interior stencils. Moreover as we have seen, compact SBP operators for the constant-coefficient case exist. Taken all together this points to the possibility that compact SBP operators for the second derivative with variable coefficients exist. Consequently we began our work to derive these operators. In the meantime Mattsson [12] derived specific instances of the operators $D_2^{(4,2,4)}(B)$ and $D^{(6,3,5)}(B)$. Our goal is to derive these operators in as general a form as possible so that we can optimize them to make them as efficient as possible. In this section we deal with solving (4) in the variable-coefficient case. We find the general solution for the $D_2^{(4,2,4)}(B)$ operator, and prove the existence of the $D_2^{(8,4,6)}(B)$, operator by determining a solution to (4) , while presenting a $D_2^{(6,3,5)}(B)$ operator that has preferable accuracy characteristics and has the potential to be optimized.

To understand the SBP property we use the variable-coefficient diffusion equation on the interval $[0, 1]$:

$$
\frac{\partial \mathcal{Q}}{\partial t} = \frac{\partial}{\partial x}\left(\beta \frac{\partial \mathcal{Q}}{\partial x}\right). \tag{8}
$$

Applying the energy method to (8) gives

$$\frac{d||\mathcal{Q}||^2}{dt} = 2\left(\beta Q\frac{\partial \mathcal{Q}}{\partial x}\right)\Big|_0^1 - 2\int_0^1 \beta\left(\frac{\partial \mathcal{Q}}{\partial x}\right)^2 dx. \tag{9}$$

The semi-discrete equations are

$$\frac{d\mathbf{q}}{dt} = H^{-1}\left\{-M + EBD_b\right\}\mathbf{q}.$$

Multiplying by $\mathbf{q}^T H$ and adding the transpose of the product gives

$$\begin{array}{rcl} \frac{d||\mathbf{q}||_H}{dt} & = & 2\mathbf{q}^T EBD_b\mathbf{q} - 2\mathbf{q}^T M\mathbf{q} \\ & = & 2\mathbf{q}^T EBD_b\mathbf{q} - 2(D\mathbf{q})^T HBD\mathbf{q} - 2\mathbf{q}^T R\mathbf{q}, \end{array} \tag{10}$$

and we can see that (10) is mimetic of the continuous case (9) within the discretization error, i.e. the R term is of the same order as the discretization error. This is easiest to see by noting that $2\mathbf{q}^T EBD_b\mathbf{q} = 2(q_N B(N,N)(D_b\mathbf{q})_N - q_0 B(1,1)(D_b\mathbf{q})_0)$ and $2(D\mathbf{q})^T BHD\mathbf{q}$ is the discrete approximation of $2\int_0^1 \beta\left(\frac{\partial \mathcal{Q}}{\partial x}\right)^2 dx$. Also note that the PSD property of M and R is required to find an energy estimate.

To solve for the operators we could use the simple method presented for the second derivative with constant coefficients. However, to prove that the resultant operator is PSD in the variable-coefficient case, we cannot resort to a parameter search but rather must rely on using either the Cholesky or the characteristic equation methods, both of which are difficult; we have yet to seriously attempt either. For the moment, we are forced to use (4) in order to ensure that M is PSD. This means that we must now solve a large system of nonlinear equations, which in some cases results in no solution or many solutions with many free parameters. The 4^{th}-order operator is presented in detail, as we can solve (4), and it results in two solutions with one and two free parameters respectively. Moreover, as before, we use the $D_2^{(4,2,4)}(B)$ operator as a template to detail how to solve these operators. The second-order operator, $D_2^{(2,1,2)}$, is well known and so we do not discuss it here, but simply present it in Appendix C.

For $D_2^{(4,2,4)}(B)$ we require $\tilde{D}_{3,4}^{(2,1,:)}$ and $\tilde{D}_{4,4}^{(2,1,:)}$, with the remaining matrices given as in the constant-coefficient case, and the C matrices being diagonal matrices with $2p$ unknowns at either boundary, the remaining diagonal entries being unity. For each of these we will give the boundary stencils as well as the interior stencils.

The $\tilde{D}_{3,4}^{(2,1,:)}$ operator has the following free variables before imposing constraints: d_{315}, d_{316}, d_{325}, d_{326}, d_{335}, d_{336}, d_{345}, d_{346}. The boundary and interior stencils are given as:

- $\tilde{D}_{3,4}^{(2,1,:)}(1,1:6)$: $(1+d_{315}+4d_{316}, 3-4d_{315}-15d_{316}, -3+6d_{315}+20d_{316}, 1-4d_{315}-10d_{316}, d_{315}, d_{316})$
- $\tilde{D}_{3,4}^{(2,1,:)}(2,1:6)$: $(-1+d_{325}+4d_{326}, 3-4d_{325}-15d_{326}, -3+6d_{325}+20d_{326}, 1-4d_{325}-10d_{326}, d_{325}, d_{326})$
- $\tilde{D}_{3,4}^{(2,1,:)}(3,1:6)$:: $(-1+d_{335}+4d_{336}, 3-4d_{335}-15d_{336}, -3+6d_{335}+20d_{336}, 1-4d_{335}-10d_{336}, d_{335}, d_{336})$
- $\tilde{D}_{3,4}^{(2,1,:)}(4,1:6)$:: $(-1+d_{345}+4d_{346}, 3-4d_{345}-15d_{346}, -3+6d_{345}+20d_{346}, 1-4d_{345}-10d_{346}, d_{345}, d_{346})$
- $\tilde{D}_{3,4}^{(2,1,:)}(j,j-2:j+2)$:: $(-\frac{1}{2}, 1, 0, -1, \frac{1}{2})$

where the notation d_{irc} refers to the (r,c) entry of the operator $\tilde{D}_{i,4}^{(2,1,:)}$.

The $\tilde{D}_{4,4}^{(2,1,:)}$ operator has the following free variables before imposing constraints $d_{416}, d_{426}, d_{436}, d_{446}$. The boundary and interior stencils are given as:

- $\tilde{D}_{4,4}^{(2,1,:)}(1,1:6)$: $(1-d_{416}, -4+5d_{416}, 6-10d_{416}, -4+10d_{416}, 1-5d_{416}, d_{416})$
- $\tilde{D}_{4,4}^{(2,1,:)}(2,1:6)$: $(1-d_{426}, -4+5d_{426}, 6-10d_{426}, -4+10d_{426}, 1-5d_{426}, d_{426})$

- $\tilde{D}_{4,4}^{(2,1,:)}(3,1:6)$: $(1-d_{436}, -4+5d4_{36}, 6-10d_{436}, -4+10d_{436}, 1-5d_{436}, d_{436})$
- $\tilde{D}_{4,4}^{(2,1,:)}(4,1:6)$: $(1-d_{446}, -4+5d_{446}, 6-10d_{446}, -4+10d_{446}, 1-5d_{446}, d_{446})$
- $\tilde{D}_{4,4}^{(2,1,:)}(j,j-2:j+2)$: $(1,-4,6,-4,1)$

Imposing the accuracy and form constraints we have a non-linear system with a total of 142 non-linear equations. On the other hand, we have 8 variables from $\tilde{D}_{3,4}^{(2,1,:)}$, 4 from $C_3^{(4)}$, 4 from $\tilde{D}_{4,4}^{(2,1,:)}$, and 4 from $C_4^{(4)}$, giving us 16 variables, so the system appears overdetermined. However, because of the chosen form of $D_2^{(2p,p,p+2)}(B)$ some of these equations are automatically satisfied, leaving 76 non-linear equations, see Table 1, and since we find solutions to the system we know that only a small number are independent. Solving the system, we get two solutions which have only 4 free parameters each. Furthermore, as with the constant-coefficient case, once we construct M, these reduce to only one and two and free parameters, respectively.

The first solution, with free parameter c_{32}, is given as:

$M(1,1) = \frac{1349}{1680}\, b_1 + \frac{59}{192}\, b_2 + \frac{1}{105}\, b_3 + \frac{1}{192}\, b_4 - \frac{1}{18}\, b_1 c_{32} + \frac{1}{18}\, c_{32}\, b_2,$

$M(1,2) = -\frac{649}{560}\, b_1 - \frac{59}{840}\, b_3 + \frac{1}{6}\, b_1 c_{32} - \frac{1}{6}\, c_{32}\, b_2,$

$M(1,3) = -\frac{89}{1680}\, b_1 + \frac{9}{280}\, b_3 + \frac{1}{18}\, b_1 c_{32} - \frac{1}{18}\, c_{32}\, b_2 + \frac{1}{24}\, b_4,$

$M(2,2) = \frac{13039}{6720}\, b_1 + \frac{3481}{6720}\, b_3 - \frac{1}{2}\, b_1 c_{32} + \frac{1}{2}\, c_{32}\, b_2,$

$M(2,3) = -\frac{1711}{1680}\, b_1 + \frac{1}{2}\, b_1 c_{32} - \frac{1}{2}\, c_{32}\, b_2 - \frac{59}{280}\, b_3,$

$M(2,4) = \frac{531}{2240}\, b_1 - \frac{531}{2240}\, b_3 - \frac{1}{6}\, b_1 c_{32} + \frac{1}{6}\, c_{32}\, b_2,$

$M(3,3) = \frac{1501}{1680}\, b_1 + \frac{59}{192}\, b_2 + \frac{113}{192}\, b_4 + \frac{1}{24}\, b_5 - \frac{1}{2}\, b_1 c_{32} + \frac{1}{2}\, c_{32}\, b_2 + \frac{129}{280}\, b_3,$

$M(3,4) = -\frac{159}{560}\, b_1 - \frac{1}{6}\, b_5 + \frac{1}{6}\, b_1 c_{32} - \frac{1}{6}\, c_{32}\, b_2 - \frac{113}{280}\, b_3 - \frac{3}{8}\, b_4,$

$M(4,4) = \frac{671}{6720}\, b_1 + \frac{5209}{6720}\, b_3 + \frac{5}{6}\, b_5 + \frac{1}{24}\, b_6 - \frac{1}{18}\, b_1 c_{32} + \frac{1}{18}\, c_{32}\, b_2 + \frac{17}{24}\, b_4.$

The second solution, with free parameters c_{32}, c_{33}, is given as:

$M(1,1) = \frac{1699}{2064}\, b_1 + \frac{59}{192}\, b_2 - \frac{11}{1032}\, b_3 + \frac{1}{192}\, b_4 - \frac{1}{18}\, b_1 c_{32} - \frac{1}{18}\, b_1 c_{33} + \frac{1}{18}\, c_{32}\, b_2 + \frac{1}{18}\, b_3 c_{33},$

$M(1,2) = -\frac{839}{688}\, b_1 - \frac{5}{516}\, b_3 + \frac{1}{6}\, b_1 c_{32} + \frac{1}{6}\, b_1 c_{33} - \frac{1}{6}\, c_{32}\, b_2 - \frac{1}{6}\, b_3 c_{33},$

Table 1: Number of equations from the form and accuracy constraints at boundary nodes for $D_2^{(4,2,4)}(B)$

Node	form constraints	accuracy constraints	automatically satisfied	net number of equations
1	8	10	9	9
2	8	10	9	9
3	10	10	9	11
4	12	10	9	13
5	14	21	15	20
6	8	21	15	14
Total	60	82	66	76

$M(1,3) = -\frac{839}{688}\, b_1 - \frac{5}{516}\, b_3 + \frac{1}{6}\, b_1 c_{32} + \frac{1}{6}\, b_1 c_{33} - \frac{1}{6}\, c_{32}\, b_2 - \frac{1}{6}\, b_3 c_{33},$

$M(1,4) = -\frac{151}{2064}\, b_1 + \frac{9}{172}\, b_3 + \frac{1}{18}\, b_1 c_{32} + \frac{1}{18}\, b_1 c_{33} - \frac{1}{18}\, c_{32}\, b_2 - \frac{1}{18}\, b_3 c_{33} + \frac{1}{2}4\, b_4,$

$M(2,2) = \frac{17519}{8256}\, b_1 + \frac{2777}{8256}\, b_3 - \frac{1}{2}\, b_1 c_{32} - \frac{1}{2}\, b_1 c_{33} + \frac{1}{2}\, c_{32}\, b_2 + \frac{1}{2}\, b_3 c_{33},$

$M(2,3) = -\frac{2477}{2064}\, b_1 + \frac{1}{2}\, b_1 c_{32} + \frac{1}{2}\, b_1 c_{33} - \frac{1}{2}\, c_{32}\, b_2 - \frac{1}{2}\, b_3 c_{33} - \frac{5}{172}\, b_3,$

$M(2,4) = \frac{819}{2752}\, b_1 - \frac{819}{2752}\, b_3 - \frac{1}{6}\, b_1 c_{32} - \frac{1}{6}\, b_1 c_{33} + \frac{1}{6}\, c_{32}\, b_2 + \frac{1}{6}\, b_3 c_{33},$

$M(3,3) = \frac{2219}{2064}\, b_0 + \frac{59}{192}\, b_1 + \frac{113}{192}\, b_3 + \frac{1}{2}4\, b_4 - \frac{1}{2}\, b_0 c_{32} - \frac{1}{2}\, b_0 c_{33} + \frac{1}{2}\, b_1 c_{32} + \frac{1}{2}\, b_2 c_{33} + \frac{12}{43}\, b_2,$

$M(3,4) = -\frac{237}{688}\, b_0 - \frac{1}{6}\, b_4 + \frac{1}{6}\, b_0 c_{32} + \frac{1}{6}\, b_0 c_{33} - \frac{1}{6}\, b_1 c_{32} - \frac{1}{6}\, b_2 c_{33} - \frac{59}{172}\, b_2 - \frac{3}{8}\, b_3,$

$M(4,4) = \frac{991}{8256}\, b_{-1} + \frac{6233}{8256}\, b_1 + \frac{5}{6}\, b_3 + \frac{1}{2}4\, b_4 - \frac{1}{18}\, b_{-1} c_{32} - \frac{1}{18}\, b_{-1} c_{33} + \frac{1}{18}\, b_0 c_{32} + \frac{1}{18}\, b_1 c_{33} + \frac{17}{24}\, b_2.$

The interior entries are given as:

$M(j, j-2) = -\frac{1}{6}\, b_{j-1} + \frac{1}{8}\, b_{j-2} + \frac{1}{8}\, b_j,$

$M(j, j-1) = -\frac{1}{6}\, b_{j-2} - \frac{1}{6}\, b_{j+1} - \frac{1}{2}\, b_{j-1} - \frac{1}{2}\, b_j,$

$M(j, j) = \frac{1}{2}4\, b_{j-2} + \frac{5}{6}\, b_{j-1} + \frac{5}{6}\, b_{j+1} + \frac{1}{2}4\, b_{j+2} + \frac{3}{/}4\, b_j,$

$M(j, j+1) = -\frac{1}{6}\, b_{j-1} - \frac{1}{6}\, b_{j+2} - \frac{1}{2}\, b_j - \frac{1}{2}\, b_{j+1},$

$M(j, j+2) = -\frac{1}{6}\, b_{j+1} + \frac{1}{8}\, b_j + \frac{1}{8}\, b_{j+2}.$

For the $D_2^{(6,3,5)}(B)$ operator, we are not as fortunate as with the $D_2^{(4,2,4)}(B)$ operator. We cannot solve the resultant system of equations with all the free variables in $D^{(6,3,5)} = 1$, $\tilde{D}_{4,5}^{(2,1,:)} = 24$, $C_4^{(5)} = 6$, $\tilde{D}_{5,5}^{(2,1,:)} = 18$, $C_5^{(5)} = 6$, and $\tilde{D}_{6,5}^{(2,1,:)} = 12$, $C_6^{(5)} = 6$, a total of 76. For the $D_2^{(6,3,5)}(B)$ operator we must now make a decision as to how to simplify the resultant system of equations so that we can attain a solution. First we can drop the accuracy and the form constraints; we will call this the no-constraints condition. We note that the equations for the no-constraints condition only include free variables from $\tilde{D}_{4,5}^{(2,1,:)}$ and $C_4^{(5)}$, and so we are free to set the remaining free variables to any choice. We set the boundary equations of the remaining matrices to the interior stencil and the non-unity values of the C matrices to zero. At boundary nodes, for the $\tilde{D}_{i,5}^{(2,1,:)}$ operators, we cannot use stencils that have smaller bandwidth than the interior stencil, since no solution can be found under any condition for such boundary operators, so in practice we either leave all the variables in the boundary nodes or we use the interior stencil. Moreover, our choice of setting the non-unity entries in the diagonal C matrices for the no-constraints derivation to zero is based upon our experience for which many of the solutions have zeros for these entries. The no-constraints operator is problematic for two reasons: first we now have an additional p nodes at each boundary that are p accurate, and second, the stencils at the boundary nodes are p wider than in the first and second derivative with constant coefficients.

We have tried to solve for just the accuracy constraints, but we find that it is impossible to solve in the general case. In order to satisfy both the accuracy and form constraints and find a solution, we must somehow simplify the system of equations. Two possibilities have lead to solutions. In the first, we systematically set boundary nodes in the $\tilde{D}_{i,e}^{(2,1,:)}$ operators to their respective interior stencils. In the second, we solve for the free variables in the first-derivative operator, $D_1^{(6,3,4)}$. From our experience with the $D_2^{(8,4,6)}(B)$ operator, we note that specifying the values of the free variables in the first derivative substantially simplifies the resultant system of equations. In fact, in that case we have been unable to solve the system under any condition without specifying the free variables of the first derivative. Still for the $D_2^{(6,3,5)}(B)$ operator we can get away with not specifying the free variables in the first derivative; instead we have been able to solve up to only having the first two boundary stencils in $\tilde{D}^{(2,1,:)}_{5,5}$ and $\tilde{D}^{(2,1,:)}_{6,5}$, set to the interior stencil while retaining the remaining free variables and imposing both the accuracy and the form constraints. This results in 71 solutions, many of which can be discarded, 9 of which we know directly have members which satisfy the PSD conditions, while another 23, potentially could satisfy the PSD condition. We have not investigated these yet, as their form is significantly more complex than the solution we present in this paper. We present one of the 9 solutions for which a PSD M exists that has a particularly simple form. The final M only has one free parameter, and the solution specifies the free parameter in the first derivative which results in an operator for the first derivative with accuracy characteristics very close to those of the first derivative optimized about minimizing the L_∞ error of the first derivative on a known test function. We summarize the various approaches to solving $D^{(6,3,5)}_2(B)$ in Table 2, where CC stands for constant-coefficient constraints, A for accuracy constraints, F for form constraints and OFD for optimized first derivative constraints.

Table 2: Solution methods for $D^{(6,3,5)}_2(B)$

Constraints	Comment
none	Many free parameters, difficult to optimize, large boundary stencil width, p accurate at $3p$ boundary nodes at either boundary
CC	Have not found solutions yet using these restrictions
A	Cannot solve without setting some boundary nodes in $D^{(2,:,:)}_i$ to respective interior stencils
A&F	Cannot solve without setting some boundary nodes in $D^{(2,:,:)}_i$ to respective interior stencils
A&F and CC	Have not found solutions yet using these restrictions
A&F and OFD	Have not found solutions yet using these restrictions
A&F, OFD, and CC	Have not found solutions yet using these restrictions

For the $D^{(8,4,6)}_2(B)$ operator we encounter even more challenges. As mentioned, we cannot even find a solution for the no-constraint case without specifying the free variables of the first derivative. For this paper we limit the presentation to a particular solution to demonstrate the existence of the operator. For simplicity we set all boundary equations for the $\tilde{D}^{(2,1,:)}_{i,6}$ operators to the interior stencil and all of the free variables in the $C^{(6)}_i$ matrices to zero, adding free variables to the $\tilde{D}^{(2,1,:)}_{5,6}$ and $C^{(6)}_5$ operators until we have a sufficient number of variables to solve the no-constraints system of equations. In this manner we obtain a unique operator, given in Appendix C.

2.6 Summary of SBP operators for the second derivative

We have covered a lot of ground in the above section and feel it important to summarize where we are and what still needs to be done. For SBP operators for the second derivative with constant coefficients we have found a novel way to circumvent deriving the operators using (4), while enforcing the PSD constraint on M. We have yet to tackle in a systematic way optimizing these operators and the relationship between optimized versions of the first and second derivatives. That is to say, in our limited numerical experimentation we have found that the optimum for the second derivative with constant coefficients uses a first-derivative operator that does not necessarily coincide with the optimum for the first derivative by itself. Although we have been unable to use information about the constant-coefficient case for the variable-coefficient case, we believe that ultimately this will be useful information in either simplifying the resultant non-linear system of equations, or, if we manage to solve for the variable-coefficient operators in the general case, as we did for the $D_2^{(4,2,4)}(B)$ operator, to simplify the choice of the free parameters that remain.

For SBP operators for the second derivative with variable coefficients, our goal has been to derive these using the general form (4) while satisfying the accuracy and form constraints. We managed to do so for the $D_2^{(4,2,4)}(B)$ case but encounter difficulties with the higher order operators. For the $D_2^{(6,3,5)}(B)$ operator, we almost manage to solve the general case with the accuracy and form constraints, having only to set the first two boundary stencils of the $\tilde{D}_{5,5}^{(2,1,:)}$ and $\tilde{D}_{6,5}^{(2,1,:)}$ matrices to their interior stencils. Finally, for the $D_2^{(8,4,6)}(B)$ operator, we were unable to solve with the accuracy and form constraints and instead limit the presentation to an operator that satisfies the no-constraint conditions and has no free parameters.

In the future, we would ideally like to solve for both the $D_2^{(6,3,5)}(B)$ and the $D_2^{(8,4,6)}(B)$ operators in the general case with the accuracy and form constraints. Baring this, we will use some combination of specifying the free parameters of the first derivative and having the operators collapse onto optimized versions of the constant-coefficient case in order to simplify the resultant system of equations.

3 Boundary conditions and dissipation model

With SBP operators it is typical to use SATs to enforce boundary conditions weakly. Moreover, as the compressible NS equations, which are nonlinear, are of interest, we require a dissipation model to stabilize the solution. The dissipation model is a modified version of that proposed by Diener et al. [9]. To explain both concepts consider the linear convection-diffusion equation with variable coefficients (see [21] for the case with $b = 1$):

$$\frac{\partial \mathcal{Q}}{\partial t} = -a\frac{\partial \mathcal{Q}}{\partial x} + \epsilon\frac{\partial}{\partial x}\left(b\frac{\partial \mathcal{Q}}{\partial x}\right), 0 \leq x \leq 1, t \geq 0$$

$$\mathcal{Q}(0,t) + \alpha b\frac{\partial \mathcal{Q}(0,t)}{\partial x} = 0, \frac{\partial \mathcal{Q}(1,t)}{\partial x} = 0,$$

$$\mathcal{Q}(x,0) = f(x),$$

$$\frac{-2\epsilon}{a} \leq \alpha \leq 0,$$

and its semi-discrete analogue with SATs and dissipation model applied,

$$\frac{d\mathbf{q}}{dt} = -aD\mathbf{q} + \epsilon D_2(b)\mathbf{q} + SAT + DISS.$$

SATs impose the boundary conditions as penalty terms; rather than imposing the boundary term exactly, they do so within the discretization error. This method has been found to be preferable to explicit enforcement of the boundary conditions. In their comparison of weakly and strongly enforced Dirchlet boundary conditions for the boundary layer solution of the advection-diffusion equation and the incompressible NS equations, Bazilevs and Hughes [36] found that weakly imposed boundary conditions resulted in faster convergence to steady state. Similarly, Eliasson et al. [37] found that weakly enforced boundary conditions for the NS equations resulted in faster convergence to steady state, suggesting that the reason for this was an improved eigenspectrum for the semi-discrete equations.

The SAT term has the following form, [21]:

$$\begin{aligned} \text{SAT} = \quad & -\frac{H^{-1}}{2}\left(\tau_L\mathbf{e}_L^T\left[q - \mathcal{Q}(0)\mathbf{e}_L + \alpha b D_b q - b\frac{\partial \mathcal{Q}(0)}{\partial x}\mathbf{e}_L\right]\right), \\ & -\frac{H^{-1}}{2}\left(\tau_R\mathbf{e}_R^T\left[bD_b q - b\frac{\partial \mathcal{Q}(1)}{\partial x}\mathbf{e}_R\right]\right). \end{aligned}$$

where $\tau_L = \frac{-2\epsilon}{\alpha}, and \tau_R = 2\epsilon$.

4 Method of Manufactured Solutions

In the method of manufactured solutions [38] a solution is assumed, and a source term is introduced such that the assumed solution satisfies the equation. For the one-dimensional linear convection-diffusion equation we have:

$\frac{\partial \mathcal{U}}{\partial t} = -\frac{\partial \mathcal{U}}{\partial x} + \frac{\partial}{\partial x}\left(b\frac{\partial \mathcal{U}}{\partial x}\right) + \mathcal{G},$

where

$\mathcal{G} = 2\epsilon\cos(x)\sin(x)e^{-t} + \cos(x)e^{-t},$

and $b = 1+\epsilon\cos(x)$, the initial conditions are $\mathcal{U}(x,0) = \sin(x)$, and the solution is given as $\mathcal{U}(x,t) = \sin(x)e^{-t}$.

5 Results

Here we present some results for the 2^{nd} to 6^{th} global order SBP operators for both compact-stencil and non-compact-stencil operators in the context of the one-dimensional linear convection-diffusion equation with the source term given in Section 4.

For the $D_2^{(4,2,4)}$ operator, we have two solutions with one and two free parameters, respectively. We perform a simple parameter search to optimize the operator with regards to the above problem. In the parameter search we use the L_2 norm as a measure of the error, looking for values of the free parameters that minimize this norm. For the first solution we find that the minimum occurs for $c_{32} = 0$. For the second solution we find that the minimum also occurs for $c_{32} = 0$, and we are left with minimizing about c_{33}. For c_{33} we find a slight dependence on the number of nodes, N, in the operator, varying between $c_{33} \in [2.020202818181819, 2.222223]$. For operators $101 \geq N \geq 25$ the dependence vanishes and we get a consistent value of $c_{33} = 2.121212909090910$, which will be used for the remaining computations.

The solution for the $D_2^{(6,3,5)}(B)$ operator we present in this paper has only one free parameter, c_{54}, while the free variable in the first derivative is specified by the solution as $\Theta_{15} = \frac{13241}{259200}$. We find a minimum for $c_{54} = 19.363363363363362$. Figure 1 shows the L_2 norm of the solution error, where the L_2 norm is computed using:

$$L_2 = \sqrt{\sum_{i=1}^{N+1} \frac{(q_{c,i} - q_{e,i})^2}{(N+1)}}, \tag{11}$$

where $q_{c,i}$ is the computed solution and $q_{e,i}$ is the exact solution at the i^{th} node. We can see from the figure that we attain or surpass the theoretical rates of convergence, except for the non-compact-stencil $D_2^{(4,1,3)}(B)$ operator, which comes very close. The compact-stencil operators not only give an additional order of accuracy but produce a global discretization error that is substantially less than that of the non-compact-stencil operators (application of the first derivative twice).

6 Conclusions and Future Work

We have presented a general framework for deriving higher-order maximally-compact-stencil SBP operators, where the interior stencil width is the same as that for the compact first derivative, for the second derivative with constant and variable coefficients. The proposed operators posses better accuracy characteristics and reduce the number of equations that need to be solved. General solutions were found for the $D_2^{(4,2,4)}(B)$ operator while a family of solutions for the $D_2^{(6,3,5)}(B)$ operator was determined, for which we presented a solution with a simple form with one free parameter that was used to optimize the operator for the linear convection-diffusion equation. Derivation of the $D_2^{(8,4,6)}(B)$ operator required specification of the free parameters in the first derivative, and we reduced the number of remaining free parameters to obtain a unique solution.

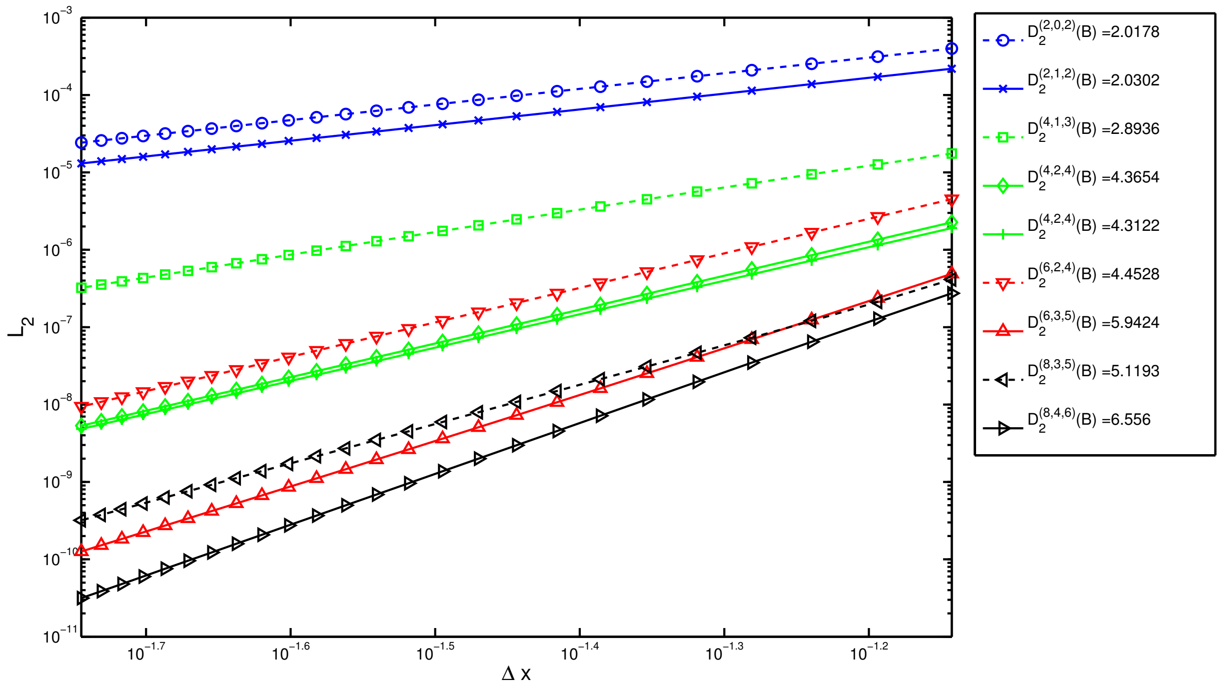

Figure 1: L_2 norm of the error for the one-dimensional linear convection-diffusion equation. Solid lines are for the compact-stencil operator, while dashed lines are for the non-compact-stencil operator. The slope of each line is given beside the operator name, and solution one for $D_2^{(4,2,4)}(B)$ is given as the green line with diamonds, while solution two is given as the green solid line with crosses.

Our study of the compact-stencil operator for the second derivative with variable coefficients, as applied to the linear convection-diffusion equation, has shown that the proposed operators behave as theoretically predicted. In line with the results of of Mattsson et al. [8], and Mattsson [12], we get $p+2$ convergence rates for the compact-stencil operators and $p+1$ for the non-compact-stencil operators. Moreover, the compact-stencil operators have a significantly smaller global error relative to the non-compact-stencil operators. In future work we intend to implement and characterize the proposed SBP operators for the compressible NS equations.

Our next steps will be to derive the $D_2^{(6,3,5)}(B)$ and $D_2^{(8,4,6)}(B)$ in the general case with the accuracy and form constraints. Given our interest in optimization, efficiency is a major priority, particularly as we are interested in optimization based on the NS equations including the effects of turbulence using either the Reynolds-averaged equations or large-eddy simulations. Deriving the operators in the general case gives us the ability to optimize the operators as to make them as efficient as possible. Moreover, since in optimization functionals are the quantity of concern, extending the dual-consistent formulation proposed by Hicken and Zingg [27] for the Euler equations to the compressible NS equations would give us additional accuracy in our computations and will be pursued in the near future.

References

[1] H.-O. Kreiss and J. Oliger. Comparison of accurate methods for the integration of hyperbolic equations. *Tellus*, 24(3):199–215, 1972.

[2] B. Swartz and B. Wendroff. The relative efficiency of finite difference and finite element methods: I hyperbolic problems and splines. *SIAM Journal on Numerical Analysis*, 11(5):979–993, 1974.

[3] D. W. Zingg. Comparison of high-accuracy finite-difference methods for linear wave propagation. *SIAM Journal on Scientific Computing*, 22(2):476–502, 2000.

[4] D. W. Zingg, S. De Rango, M. Nemec, and T. H. Pulliam. Comparison of several spatial discretizations for the Navier-Stokes equations. *Journal of Computational Physics*, 160(2):683–704, 2000.

[5] S. De Rango and D. W. Zingg. Higher-order spatial discretization for turbulent aerodynamic computations. *AIAA Journal*, 39(7):1296–1304, 2001.

[6] H.-O Kreiss and G. Scherer. *Mathematical aspects of finite elements in partial differential equations*, chapter Finite element and finite difference methods for hyperbolic partial differential equations. Academic Press, New York/London, 1974.

[7] B. Strand. Summation by parts for finite difference approximations for d/dx. *Journal of Computational Physics*, 110(1):47–67, 1994.

[8] K. Mattsson, M. Svärd, and J. Nordström. Stable and accurate artificial dissipation. *Journal of Scientific Computing*, 21(1):57–79, 2004.

[9] P. Diener, E. N. D., E. Schnetter, and M. Tiglio. Optimized high-order derivative and dissipation operators satisfying summation by parts, and applications in three-dimensional mulit-block evolutions. *Journal of Scientific Computing*, 32(1):109–145, 2007.

[10] K. Mattsson and J. Nordström. Summation by parts operators for finite difference approximations of second derivatives. *Journal of Computational Physics*, 199:503–540, 2004.

[11] K. Mattsson, M. Svard, and M. Shoeybi. Stable and accurate schemes for the compressible Navier–Stokes equations. *Journal of Computational Physics*, 227(4):2293–2316, 2008.

[12] K. Mattsson. Summation by parts operators for finite difference approximations of second-derivatives with variable coefficients. *Journal of Scientific Computing*, 51(3):650–682, 2011.

[13] D. Funaro and D. Gottlieb. A new method of imposing boundary conditions in pseudospectral approximations of hyperbolic equations. *Mathematics of Computation*, 51(184):599–613, 1988.

[14] M. H. Carpenter, D. Gottlieb, and S. Abarbanel. Time-stable boundary conditions for finite-difference schemes solving hyperbolic systems: methodology and application to high-order compact schemes. *Journal of Computational Physics*, 111(2):220–236, 1994.

[15] J. S. Hesthaven. A stable penalty method for the compressible Navier-Stokes equations: III multidimensional domain decomposition schemes. *SIAM Journal on Scientific Computing*, 20(1), 1988.

[16] M. H. Carpenter, J. Nordström, and D. Gottlieb. A stable and conservative interface treatment of arbitrary spatial accuracy. *Journal of Computational Physics*, 148(2):341–365, 1999.

[17] J. Nordström and M. H. Carpenter. Boundary and interface conditions for high order finite difference methods applied to the Euler and Navier-Stokes equations. *Journal of Computational Physics*, 148(2):621–645, 1999.

[18] J. Nordström and M. H. Carpenter. High-order finite-difference methods, multidimensional linear problems, and curvilinear coordinates. *Journal of Computational Physics*, 173(1):149–174, 2001.

[19] M. Svärd, M. H. Carpenter, and J. Nordström. A stable high-order finite difference scheme for the compressible Naiver-Stokes equations, far-field boundary conditions. *Journal of Computational Physics*, 225(1):1020–1038, 2007.

[20] M. Svärd and J. Nordström. A stable high-order finite difference scheme for the compressible Navier–Stokes equations: No-slip wall boundary conditions. *Journal of Computational Physics*, 227(10):4805–4824, 2008.

[21] K. Mattsson. Boundary procedures for summation-by-parts operators. *Journal of Scientific Computing*, 1(133-153), 2003.

[22] J. Nordström, J. Gong, E. van der Weide, and M. Svärd. A stable and conservative high order multi-block method for the compressible Navier-Stokes equations. *Journal of Computational Physics*, 228(24):9020–9035, 2009.

[23] M. H. Carpenter, J. Nordström, and D. Gottlieb. A stable and conservative interface treatment of arbitrary spatial accuracy. *Journal of Computational Physics*, 148(2):341–365, 1999.

[24] J. Nordström and R. Gustafsson. High order finite difference approximations of electromagnetic wave propagation close to material discontinuities. *Journal of Scientific Computing*, 18(2):215–234, 2003.

[25] M. Svärd. On coordinate transformations for summation-by-parts operators. *Journal of Scientific Computing*, 20(1):29–42, 2004.

[26] B. Gustafsson. The convergence rate for difference approximations to general mixed initial boundary value problems. *SIAM Journal on Numerical Analysis*, 18(2):179–190, 1981.

[27] J. E. Hicken and D. W. Zingg. The role of dual consistency in functional accuracy: Error estimation and superconvergence. *AIAA paper 2011-3070*, 2011.

[28] J. E. Hicken and D. W. Zingg. A parallel Newton- Krylov solver for the euler equations discretized using simultaneous approximation terms. *AIAA Journal*, 46(11):2773–2786, 2008.

[29] S. Dias and D. W. Zingg. A high-order parallel Newton-Krylov flow solver for the euler equations. *AIAA paper*, 2009-3657, 2009.

[30] J. E. Hicken and D. W. Zingg. Superconvergent functional estimates from summation-by- parts finite-difference discretizations. *SIAM Journal on Scientific Computing*, 33(2):893–922, 2011.

[31] P. Olsson. Summation by parts, projections, and stability. i. *Mathematics of Computation*, 64(211):1035–1065, 1995.

[32] M. Gerritsen and P. Olsson. Designing an efficient solution strategy for fluid flows: 1. a stable high order finite difference scheme and sharp shock resolution for the euler equations. *Journal of Computational Physics*, 129(2):245–262, 1996.

[33] R. Kamakoti and C. Pantano. High-order narrow stencil finite-difference approxmations of second-derivatives involving variable coefficients. *SIAM Journal on Scientific Computing*, 31(6):4222–4243, 2009.

[34] R. A. Horn and C. R. Johnson. *Matrix Analysis*. Cambridge Universiyt Press, 1985.

[35] K. Mattsson. Summation by parts operators for finite difference approximations of second-derivatives with variable coefficients. Technical report, Department of Information Technology, Uppsala University, October 2010.

[36] Y. Bazilevs and T. J. R. Hughes. Weak imposition of Dirichlet boundary conditions in fluid mechanics. *Computers & Fluids*, 36(1):12–26, 2007.

[37] P. Eliasson, S. Eriksson, and J. Nordström. The influence of weak and strong solid wall boundary conditions on the convergence to steady-state of the Navier-Stokes equations. *AIAA Paper 2009-3551*, 2009.

[38] C. J. Roy, C. C. Nelson, T. M. Smith, and C. C. ober. Verification of Euler/Navier-Stokes codes using the method of manufactured solutions. *International journal for numerical methods in fluids*, 44(6):599–620, 2004.

A First-derivative operators

Using the approach for deriving the first derivative SBP operators given in the text, we present them below.

$D_1^{(2,1,2)}$: $H = h \times \operatorname{diag}\left(\frac{1}{2}, 1, \ldots, 1, \frac{1}{2}\right)$,

$$\Theta = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{2} & 0 & \frac{1}{2} \\ & & & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}.$$

$D_1^{(4,2,3)}$: $H = h \times \operatorname{diag}\left(\frac{17}{48}, \frac{59}{48}, \frac{43}{48}, \frac{49}{48}, 1, \ldots, 1, \frac{49}{48}, \frac{43}{48}, \frac{59}{48}, \frac{17}{48}\right)$

$$\Theta = \begin{bmatrix} -\frac{1}{2} & \frac{59}{96} & -\frac{1}{12} & -\frac{1}{32} & & & & & & & \\ -\frac{59}{96} & 0 & \frac{59}{96} & 0 & & & & & & & \\ \frac{1}{12} & -\frac{59}{96} & 0 & \frac{59}{96} & -\frac{1}{12} & & & & & & \\ \frac{1}{32} & 0 & -\frac{59}{96} & 0 & \frac{2}{3} & -\frac{1}{12} & & & & & \\ & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & & & & \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\ & & & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} & & \\ & & & & & \frac{1}{12} & -\frac{2}{3} & 0 & \frac{59}{96} & 0 & -\frac{1}{32} \\ & & & & & & \frac{1}{12} & -\frac{59}{96} & 0 & \frac{59}{96} & -\frac{1}{12} \\ & & & & & & & 0 & -\frac{59}{96} & 0 & \frac{59}{96} \\ & & & & & & & \frac{1}{32} & \frac{1}{12} & -\frac{59}{96} & \frac{1}{2} \end{bmatrix}$$

$D_1^{(6,3,4)}$: $H = h \times \operatorname{diag}\left(\frac{13649}{43200}, \frac{12013}{8640}, \frac{2711}{4320}, \frac{5359}{4320}, \frac{7877}{8640}, \frac{43801}{43200}, 1, \ldots, 1, \frac{43801}{43200}, \frac{7877}{8640}, \frac{5359}{4320}, \frac{2711}{4320}, \frac{12013}{8640}, \frac{13649}{43200}\right)$

$$
\Theta\left[\begin{array}{ccccccccccccccc}
\theta_{11} & \theta_{12} & \theta_{13} & \theta_{14} & \theta_{15} & \theta_{16} & & & & & & & & & \\
-\theta_{12} & 0 & \theta_{23} & \theta_{24} & \theta_{25} & \theta_{26} & & & & & & & & & \\
-\theta_{13} & -\theta_{23} & 0 & \theta_{34} & \theta_{35} & \theta_{36} & & & & & & & & & \\
-\theta_{14} & -\theta_{24} & -\theta_{34} & 0 & \theta_{45} & \theta_{46} & \frac{1}{60} & & & & & & & & \\
-\theta_{15} & -\theta_{25} & -\theta_{35} & -\theta_{45} & 0 & \theta_{56} & -\frac{3}{20} & \frac{1}{60} & & & & & & & \\
-\theta_{16} & -\theta_{26} & -\theta_{36} & -\theta_{46} & -\theta_{56} & 0 & \frac{3}{4} & -\frac{3}{20} & \frac{1}{60} & & & & & & \\
 & & & -\frac{1}{60} & \frac{3}{20} & -\frac{3}{4} & 0 & \frac{3}{4} & -\frac{3}{20} & \frac{1}{60} & & & & & \\
 & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & & & & \\
 & & & & & -\frac{1}{60} & \frac{3}{20} & -\frac{3}{4} & 0 & \frac{3}{4} & -\frac{3}{20} & \frac{1}{60} & & & \\
 & & & & & & -\frac{1}{60} & \frac{3}{20} & -\frac{3}{4} & 0 & \theta_{56} & \theta_{46} & \theta_{36} & \theta_{26} & \theta_{16} \\
 & & & & & & & -\frac{1}{60} & \frac{3}{20} & -\theta_{56} & 0 & \theta_{45} & \theta_{35} & \theta_{25} & \theta_{15} \\
 & & & & & & & & -\frac{1}{60} & -\theta_{46} & -\theta_{45} & 0 & \theta_{34} & \theta_{24} & \theta_{14} \\
 & & & & & & & & & -\theta_{36} & -\theta_{35} & -\theta_{34} & 0 & \theta_{23} & \theta_{13} \\
 & & & & & & & & & -\theta_{26} & -\theta_{25} & -\theta_{24} & \theta_{23} & 0 & \theta_{12} \\
 & & & & & & & & & -\theta_{16} & -\theta_{15} & -\theta_{14} & \theta_{13} & \theta_{12} & -\theta_{11}
\end{array}\right]
$$

where,

$\theta_{11} = -\frac{1}{2},\ \theta_{12} = \frac{224881}{345600} - \frac{1}{4}\ \theta_{15},\ \theta_{13} = -\frac{10073}{129600} + \theta_{15},\ \theta_{14} = -\frac{16033}{172800} - \frac{3}{2}\,\theta_{15},\ \theta_{16} = -\frac{1}{4}\,\theta_{15} + \frac{20539}{1036800},$

$\theta_{23} = \frac{49967}{103680} - \frac{5}{2}\,\theta_{15},\ \theta_{24} = \frac{187}{960} + 5\,\theta_{15},\ \theta_{25} = \frac{383}{13824} - \frac{15}{4}\,\theta_{15},\ \theta_{26} = \theta_{15} - \frac{1741}{32400},$

$\theta_{34} = \frac{28279}{51840} - 5\,\theta_{15},\ \theta_{35} = 5\,\theta_{15} - \frac{4651}{25920},\ \theta_{36} = -\frac{3}{2}\,\theta_{15} + \frac{2197}{57600},$

$\theta_{45} = -\frac{5}{2}\,\theta_{15} + \frac{25157}{34560},\ \theta_{46} = \theta_{15} - \frac{12581}{129600},$

$\theta_{56} = -\frac{1}{4}\,\theta_{15} + \frac{147127}{207360},$

$D_1^{(8,4,5)}$: $H=\mathrm{diag}\left(\frac{1498139}{5080320}, \frac{1107307}{725760}, \frac{20761}{80640}, \frac{1304999}{725760}, \frac{299527}{725760}, \frac{103097}{80640}, \frac{670091}{725760}, \frac{5127739}{5080320}, 1, \ldots, 1, \frac{5127739}{5080320}, \frac{670091}{725760}, \frac{103097}{80640}, \frac{299527}{725760}, \frac{1304999}{725760}, \frac{20761}{80640}, \frac{1107307}{725760}, \frac{1498139}{5080320}\right)$

$\theta_{11} = -\frac{1}{2},\ \theta_{12} = -\frac{114877129}{6773760} + \frac{1}{5}\,\theta_{27} + 5\,\theta_{68} + 24\,\theta_{78},\ \theta_{13} = \frac{571884877}{6773760} - \theta_{27} - 24\,\theta_{68} - 115\,\theta_{78},$

$\theta_{14} = -\frac{9637446191}{60963840} + 2\,\theta_{27} + 215\,\theta_{78} + 45\,\theta_{68},\ \theta_{15} = \frac{236230403}{1693440} - 2\,\theta_{27} - 40\,\theta_{68} - 190\,\theta_{78},$

$\theta_{16} = -\frac{1417763}{27648} + \theta_{27} + 15\,\theta_{68} + 70\,\theta_{78},\ \theta_{17} = -\frac{6688951}{8709120} - \frac{1}{5}\,\theta_{27} + \theta_{78},\ \theta_{18} = \frac{24839327}{6773760} - \theta_{68} - 5\,\theta_{78},$

$\theta_{23} = -\frac{119306357}{483840} + 3\,\theta_{27} + 70\,\theta_{68} + 336\,\theta_{78},\ \theta_{24} = \frac{149409773}{241920} - 8\,\theta_{27} - 175\,\theta_{68} - 840\,\theta_{78},\ \theta_{25} = -\frac{5373215293}{8709120} + 9\,\theta_{27} + 175\,\theta_{68} + 840\,\theta_{78},$

$\theta_{26} = \frac{119306357}{483840} - \frac{24}{5}\,\theta_{27} - 70\,\theta_{68} - 336\,\theta_{78},\ \theta_{28} = -\frac{536324953}{30481920} + 5\,\theta_{68} + 24\,\theta_{78},\ \theta_{34} = -\frac{40075829}{53760} + 10\,\theta_{27} + 210\,\theta_{68} + 1015\,\theta_{78},$

$\theta_{35} = \frac{970678259}{967680} - 15\,\theta_{27} - 280\,\theta_{68} - 1365\,\theta_{78},\ \theta_{36} = -\frac{3559543}{7680} + 9\,\theta_{27} + 126\,\theta_{68} + 630\,\theta_{78},\ \theta_{37} = \frac{1298651}{120960} - 2\,\theta_{27} - 14\,\theta_{78},$

$\theta_{38} = \frac{7439833}{225792} - 10\,\theta_{68} - 45\,\theta_{78},\ \theta_{45} = -\frac{622544147}{967680} + 10\,\theta_{27} + 175\,\theta_{68} + 875\,\theta_{78},\ \theta_{46} = \frac{9523751}{23040} - 8\,\theta_{27} - 105\,\theta_{68} - 560\,\theta_{78},$

$\theta_{47} = -\frac{4165723}{155520} + 2\,\theta_{27} + 35\,\theta_{78},\ \theta_{48} = -\frac{19764155}{677376} + 10\,\theta_{68} + 40\,\theta_{78},\ \theta_{56} = 3\,\theta_{27} - \frac{30014249}{193536} + 35\,\theta_{68} + 210\,\theta_{78},$

$\theta_{57} = \frac{245071}{9216} - \theta_{27} - 35\,\theta_{78},\ \theta_{58} = \frac{657798011}{60963840} - 5\,\theta_{68} - 15\,\theta_{78},\ \theta_{67} = -\frac{240463}{24192} + \frac{1}{5}\,\theta_{27} + 14\,\theta_{78}$

B SBP operators for the second derivative with constant coefficients

$D_2^{(2,1,2)}: M_{11} = 1,\ M_{12} = -1,\ M_{j,j-1} = -1,\ M_{j,j} = 2,\ M_{j,j} = -1$

$\tilde{D}_1^{(:,2,:)}(11) = -\tilde{D}_1^{(:,2,:)}(N+1,N+1) = -\frac{3}{2}, \tilde{D}_1^{(:,2,:)}(12) = -\tilde{D}_1^{(:,2,:)}(N+1,N) = 2,$

$\tilde{D}_1^{(:,2,:)}(13) = -\tilde{D}_1^{(:,2,:)}(N+1,N-1) = -\frac{1}{2}$

$D_2^{(4,2,4)}:\ M_{11} = \frac{9}{8},\ M_{12} = -\frac{59}{48},\ M_{13} = \frac{1}{12},\ M_{14} = \frac{1}{48},\ M_{22} = \frac{59}{24},\ M_{23} = -\frac{59}{48},\ M_{24} = 0,\ M_{33} = \frac{55}{24},$

$M_{34} = -\frac{59}{48},\ M_{44} = \frac{59}{24},\ M_{j-2} = \frac{1}{12},\ M_{j-1} = -\frac{4}{3},\ M_j = \frac{5}{2},\ M_{j+1} = -\frac{4}{3},\ M_{j+2} = \frac{1}{12}$

$\tilde{D}_1^{(:,3,:)}(11) = -\tilde{D}_1^{(:,3,:)}(N+1,N+1) = -\frac{11}{6},\ \tilde{D}_1^{(:,3,:)}(12) = -\tilde{D}_1^{(:,3,:)}(N+1,N) = 3,$

$\tilde{D}_1^{(:,3,:)}(13) = -\tilde{D}_1^{(:,3,:)}(N+1,N-1) = -\frac{3}{2},\ \tilde{D}_1^{(:,3,:)}(14) = -\tilde{D}_1^{(:,3,:)}(N+1,N-2) = \frac{1}{2}$

$D_2^{(6,3,5)}$: Optimized values $\theta_{15} = -0.007650765076508$, $R4_{16} = 63.636363636363626$, $R5_{16} = -83.838383838383834$ and $R6_{16} = 59.595959595959584$ $M_{11} = \frac{261868392627750324 79}{22371314363653896000} + \frac{107839124700805815409}{93820217467072685005}\,\theta_{15} - \frac{5572523608171200}{1374755915701849}\,{\theta_{15}}^2 - \frac{1}{80}\,R4_{16} - \frac{1}{100}\,R5_{16} - \frac{1}{720}\,R6_{16},$

$M_{12} = -\frac{700922139910644370 97}{53691154472769350400} - \frac{107839124700805815409}{18764043493414537001}\,\theta_{15} + \frac{27862618040856000}{1374755915701849}\,{\theta_{15}}^2 + \frac{1}{16}\,R4_{16} + \frac{1}{20}\,R5_{16} + \frac{1}{144}\,R6_{16},$

$M_{13} = \frac{2305370763895992 79}{26845577236384675 20} + \frac{215678249401611630818}{18764043493414537001}\,\theta_{15} - \frac{557252360817120 00}{1374755915701849}\,{\theta_{15}}^2 - \frac{1}{8}\,R4_{16} - \frac{1}{10}\,R5_{16} - \frac{1}{72}\,R6_{16},$

$M_{14} = \frac{480573607038734353}{89485257454615584 00} - \frac{215678249401611630818}{18764043493414537001}\,\theta_{15} + \frac{55725236081712000}{1374755915701849}\,{\theta_{15}}^2 + \frac{1}{8}\,R4_{16} + \frac{1}{10}\,R5_{16} + \frac{1}{72}\,R6_{16},$

$M_{15} = \frac{107839124700805815409}{18764043493414537001}\,\theta_{15} + \frac{6838481746435627}{16778485772740422 00} - \frac{27862618040856000}{1374755915701849}\,{\theta_{15}}^2 - \frac{1}{16}\,R4_{16} - \frac{1}{20}\,R5_{16} - \frac{1}{144}\,R6_{16},$

$M_{16} = -\frac{107839124700805815409}{93820217467072685005}\,\theta_{15} - \frac{2346074127529863073}{26845577236384675 2000} + \frac{5572523608171200}{1374755915701849}\,{\theta_{15}}^2 + \frac{1}{80}\,R4_{16} + \frac{1}{100}\,R5_{16} + \frac{1}{720}\,R6_{16}$ $M_{22} = \frac{6636327825578494873}{26845577236384675 20} + \frac{539195623504029077045}{18764043493414537001}\,\theta_{15} - \frac{139313090204280000}{1374755915701849}\,{\theta_{15}}^2 - \frac{5}{16}\,R4_{16} - \frac{1}{4}\,R5_{16} - \frac{5}{144}\,R6_{16},$

$M_{23} = -\frac{1797986189259347647}{1789705149092311680} - \frac{1078391247008058154090}{18764043493414537001}\,\theta_{15} + \frac{278626180408560000}{1374755915701849}\,{\theta_{15}}^2 + \frac{5}{8}\,R4_{16} + \frac{1}{2}\,R5_{16} + \frac{5}{72}\,R6_{16},$

$M_{24} = -\frac{413513765307439787}{26845577236384675 20} + \frac{1078391247008058154090}{18764043493414537001}\,\theta_{15} - \frac{278626180408560000}{1374755915701849}\,{\theta_{15}}^2 - \frac{5}{8}\,R4_{16} - \frac{1}{2}\,R5_{16} - \frac{5}{72}\,R6_{16},$

$M_{25} = -\frac{539195623504029077045}{18764043493414537001}\,\theta_{15} + \frac{139313090204280000}{1374755915701849}\,{\theta_{15}}^2 - \frac{4171696890637049 29}{10738230894553870080} + \frac{5}{16}\,R4_{16} + \frac{1}{4}\,R5_{16} + \frac{5}{144}\,R6_{16},$

$M_{26} = \frac{107839124700805815409}{18764043493414537001}\,\theta_{15} + \frac{692236211975953 93}{22371314363653896 00} - \frac{27862618040856000}{1374755915701849}\,{\theta_{15}}^2 - \frac{1}{16}\,R4_{16} - \frac{1}{20}\,R5_{16} - \frac{1}{144}\,R6_{16}$

$M_{33} = \frac{127829446458355505}{67113943090961688} + \frac{2156782494016116308180}{18764043493414537001}\,\theta_{15} - \frac{557252360817120000}{1374755915701849}\,{\theta_{15}}^2 - \frac{5}{4}\,R4_{16} - R5_{16} - \frac{5}{36}\,R6_{16}\ ,$

$M_{34} = -\frac{3147712892227461013}{26845577236384675 20} - \frac{2156782494016116308180}{18764043493414537001}\,\theta_{15} + \frac{557252360817120000}{1374755915701849}\,{\theta_{15}}^2 + \frac{5}{4}\,R4_{16} + R5_{16} + \frac{5}{36}\,R6_{16},$

$M_{35} = \frac{1078391247008058154090}{18764043493414537001}\,\theta_{15} - \frac{278626180408560000}{1374755915701849}\,{\theta_{15}}^2 + \frac{197041321020116971}{894852574546155840} - \frac{5}{8}\,R4_{16} - \frac{1}{2}\,R5_{16} - \frac{5}{72}\,R6_{16},$

$M_{36} = -\frac{2156782494016116308l8}{18764043493414537001}\,\theta_{15} - \frac{180293443335375817}{536911544727693504O} + \frac{557252360817120O0}{1374755915701849}\,{\theta_{15}}^2 + \frac{1}{8}\,R4_{16} + \frac{1}{10}\,R5_{16} + \frac{1}{72}\,R6_{16}$

$M_{44} = \frac{12468941238494581}{4660690492427895} + \frac{21567824940161163081 80}{18764043493414537001}\,\theta_{15} - \frac{557252360817120000}{1374755915701849}\,{\theta_{15}}^2 - \frac{5}{4}\,R4_{16} - R5_{16} - \frac{5}{36}\,R6_{16},$

$M_{45} = -\frac{1078391247008058154090}{18764043493414537001}\,\theta_{15} + \frac{278626180408560000}{1374755915701849}\,{\theta_{15}}^2 - \frac{1607086159417302073}{1073823089455387008} + \frac{5}{8}\,R4_{16} + \frac{1}{2}\,R5_{16} + \frac{5}{72}\,R6_{16},$

$M_{46} = \frac{2156782494016116308 18}{18764043493414537001}\,\theta_{15} + \frac{1412441198725977743}{13422788618192337600} - \frac{55725236081712000}{1374755915701849}\,{\theta_{15}}^2 - \frac{1}{8}\,R4_{16} - \frac{1}{10}\,R5_{16} - \frac{1}{72}\,R6_{16}$

$M_{55} = -\frac{139313090204280000}{1374755915701849}\,{\theta_{15}}^2 + \frac{6967547563240370611}{2684557723638467520} + \frac{5391956235040290770 45}{18764043493414537001}\,\theta_{15} - \frac{5}{16}\,R4_{16} - \frac{1}{4}\,R5_{16} - \frac{5}{144}\,R6_{16},$

$M_{56} = \frac{27862618040856000}{1374755915701849}\,{\theta_{15}}^2 - \frac{1078391247008058154 09}{18764043493414537001}\,\theta_{15} - \frac{8489912257066819361}{5965683830307705600} + \frac{1}{16}\,R4_{16} + \frac{1}{20}\,R5_{16} + \frac{1}{144}\,R6_{16}$

$M_{66} = -\frac{5572523608171200}{1374755915701849}\,{\theta_{15}}^2 + \frac{1078391247008058154 09}{93820217467072685005}\,\theta_{15} + \frac{1805623184876053727 87}{67113943090961688000} - \frac{1}{80}\,R4_{16} - \frac{1}{100}\,R5_{16} - \frac{1}{720}\,R6_{16}$

$M_{j-3} = -\frac{1}{90}, M_{j-2} = \frac{3}{20}, M_{j-1} = -\frac{3}{2}, M_j = \frac{49}{18}, M_{j+1} = -\frac{3}{2}, M_{j+2} = \frac{3}{20}, M_{j+3} = -\frac{1}{90},$

$\tilde{D}_1(11) = -D_{b(N+1,N+1)} = -\frac{25}{12}, \tilde{D}_1^{(:,4,:)}(12) = -\tilde{D}_1^{(:,4,:)}(N+1,N) = 4,$

$\tilde{D}_1^{(:,4,:)}(13) = -\tilde{D}_1^{(:,4,:)}(N+1,N-1) = -3, \tilde{D}_1^{(:,4,:)}(14) = -\tilde{D}_1^{(:,4,:)}(N+1,N-2) = \frac{4}{3}, \tilde{D}_1^{(:,4,:)}(15) = -\tilde{D}_1^{(:,4,:)}(N+1,N-2) = -\frac{1}{4}$

$D_2^{(8,4,6)}$: Given space limitations, we present how to construct the required matrices for deriving the $D_2^{(8,4,6)}$ operator. The operator is constructed as

$$D_2^{(8,4,6)} = H^{-1}\left\{-\left(D_1^{(8,4,5)}\right)^T H D_1^{(8,4,5)} - \frac{1}{350(h)}R_5^{(6)} - \frac{1}{252(h)}R_6^{(6)} - \frac{1}{980(h)}R_7^{(6)} - \frac{1}{11200(h)}R_8^{(6)} + \frac{1}{h}E\tilde{D}_1^{(:,5,:)}\right\}.$$

Each of the matrices R_5, R_6, R_7, and R_8 is symmetric and has a box that is 12×12 with unknown coefficients, while the remaining entries are defined by the interior stencil, which is as follows:

$$R_5^{(6)}(j, j-8:j+8) = \left[-\frac{1}{16}, \frac{1}{2}, -\frac{7}{4}, \frac{7}{2}, -\frac{17}{4}, \frac{5}{2}, \frac{7}{4}, -\frac{13}{2}, \frac{69}{8}, -\frac{13}{2}, \frac{7}{4}, \frac{5}{2}, -\frac{17}{4}, \frac{7}{2}, -\frac{7}{4}, \frac{1}{2}, -\frac{1}{16}\right],$$

$$R_6^{(6)}(j, j-8:j+8) = \left[\frac{9}{100}, -\frac{21}{25}, \frac{17}{5}, -\frac{39}{5}, \frac{57}{5}, -\frac{313}{25}, \frac{363}{25}, -\frac{99}{5}, \frac{231}{10}, -\frac{99}{5}, \frac{363}{25}, -\frac{313}{25}, \frac{57}{5}, -\frac{39}{5}, \frac{17}{5}, -\frac{21}{25}, \frac{9}{100}\right],$$

$$R_7^{(6)}(j, j-8:j+8) = \left[-\frac{1}{4}, 3, -16, 49, -91, 91, 0, -143, \frac{429}{2}, -143, 0, 91, -91, 49, -16, 3, -\frac{1}{4}\right],$$

$$R_8^{(6)}(j, j-8:j+8) = [1, -16, 120, -560, 1820, -4368, 8008, -11440, 12870, -11440, 8008, -4368, 1820, -560, 120, -16, 1].$$

$\tilde{D}_1^{(:,5,:)}(1,1) = -\tilde{D}_1^{(:,5,:)}(N,N) = -\frac{4723}{2100},\ \tilde{D}_1^{(:,5,:)}(1,2) = -\tilde{D}_1^{(:,5,:)}(N,N-1) = \frac{839}{175},$

$\tilde{D}_1^{(:,5,:)}(1,3) = -\tilde{D}_1^{(:,5,:)}(N,N-2) = -\frac{157}{35},\ \tilde{D}_1^{(:,5,:)}(1,4) = -\tilde{D}_1^{(:,5,:)}(N,N-3) = \frac{278}{105},$

$\tilde{D}_1^{(:,5,:)}(1,5) = -\tilde{D}_1^{(:,5,:)}(N,N-4) = -\frac{103}{140},\ \tilde{D}_1^{(:,5,:)}(1,6) = -\tilde{D}_1^{(:,5,:)}(N,N-5) = -\frac{1}{175},$

$\tilde{D}_1^{(:,5,:)}(1,7) = -\tilde{D}_1^{(:,5,:)}(N,N-6) = \frac{6}{175},$

C SBP operators for the second derivative with variable coefficients

$D_2^{(4,2,4)}(B)$: This is a well known operator and can be derived in multiple ways. Here we present the final operator:

$$M(1,1) = \frac{1}{2}b_1 + \frac{1}{2}b_2, M(1,2) = -\frac{1}{2}b_1 - \frac{1}{2}b_2, M(2,2) = \frac{1}{2}b_1 + b_2 + \frac{1}{2}b_3$$

with the interior stencil given as

$$M(j,j-1) = -\frac{1}{2}b_{j-1} - \frac{1}{2}b_j, M(j,j) = \frac{1}{2}b_{j-1} + b_j + \frac{1}{2}b_{j+1}, M(j,j+1) = -\frac{1}{2}b_j - \frac{1}{2}b_{j+1}.$$

For the $D_2^{(6,3,5)}(B)$ operator $\Theta_{15} = \frac{13241}{259200}$, while the entries in M are as follows:

$$M(1,1) = \frac{10800}{13649}\,b_1 + \frac{4040445610095295034233695737842391292922 5841}{1216424645066600985452692122732524783080320 00}\,b_2 + \frac{1907161}{1686458880}\,b_3 + \frac{40904803}{3086784000}\,b_4 + \frac{175324081}{27659232000}\,b_5 + \frac{13315201}{17175628800}\,b_6 + \frac{1}{100}\,b_4 c_{54}$$

$$M(1,2) = -\frac{330701}{327576}\,b_1 - \frac{8453101}{562152960}\,b_3 - \frac{3625633}{370414080}\,b_4 - \frac{74983783}{3687897600}\,b_5 - \frac{835621}{2862604800}\,b_6 - \frac{119027533331695454978098162209404568901454 3}{973139716053280788362153698186019826464256 0}\,b_2 - 1/20\,b_4 c_{54}$$

$$M(1,3) = \frac{6905}{163788}\,b_1 - \frac{305008109078185925192727408367440760163}{448699610869273694375762494552757205120 0}\,b_2 - \frac{138751201}{926035200}\,b_4 + \frac{17385433}{1843948800}\,b_5 - \frac{485317}{114504192}\,b_6 + 1/10\,b_4 c_{54}$$

$$M(1,4) = \frac{14637}{54596}\,b_1 - \frac{1837135093642846375736148179648459011119709}{1216424645066600985452692122732524783080320 0}\,b_2 + \frac{10383739}{843229440}\,b_3 + \frac{309031699}{5531846400}\,b_5 + \frac{27436831}{8587814400}\,b_6 - 1/10\,b_4 c_{54} + \frac{234593}{1929240}\,b_4$$

$$M(1,5) = -\frac{13241}{163788}\,b_1 - \frac{6721147444890706745970758310604197051665 71}{2432849290133201970905384245465049566160640 0}\,b_2 + \frac{1813253}{562152960}\,b_3 + \frac{3625633}{370414080}\,b_4 + \frac{20335877}{1908403200}\,b_6 - \frac{251579}{6402600}\,b_5 + 1/20\,b_4 c_{54}$$

$$M(1,6) = -\frac{3649}{327576}\,b_1 + \frac{8135781929986216531358207073417574233645 13}{2211681172848365428095803859513681423782400 0}\,b_2 - \frac{183673}{112430592}\,b_3 + \frac{138751201}{9260352000}\,b_4 - \frac{73792093}{6146496000}\,b_5 - \frac{3649}{361440}\,b_6 - \frac{1}{100}\,b_4 c_{54}$$

$$M(2,2) = \frac{37466641}{187384320}\,b_3 - \frac{337141319}{3333726720}\,b_4 + \frac{32069569}{491719680}\,b_5 + \frac{52441}{477100800}\,b_6 + \frac{109363151401}{84907699200}\,b_1 + \frac{3688468654513792415289891494095994233163053}{9731397160532807883621536981860198264642560}\,b_2 + 1/4\,b_4 c_{54}$$

$$M(2,3) = \frac{217516705}{333372672}\,b_4 - \frac{7435519}{245859840}\,b_5 + \frac{30457}{19084032}\,b_6 - \frac{456698081}{8490769920}\,b_1 - \frac{5258430993887171086960069633794762158 81}{1794798443477094777503049978211028820480}\,b_2 - 1/2\,b_4 c_{54}$$

$$M(2,4) = -\frac{46023799}{281076480}\,b_3 - \frac{132168757}{737579520}\,b_5 - \frac{1721851}{1431302400}\,b_6 - \frac{1613490179}{4717094400}\,b_1 - \frac{8373473696281682519401417386524741906562 71}{4865698580266403941810768490930099132321280}\,b_2 + 1/2\,b_4 c_{54} - \frac{139252}{241155}\,b_4$$

$$M(2,5) = -\frac{8036873}{187384320}\,b_3 + \frac{337141319}{3333726720}\,b_4 - \frac{1276217}{318067200}\,b_6 + \frac{4378811941}{42453849600}\,b_1 + \frac{3100255381699148585555158355026708402565933}{9731397160532807883621536981860198264642560}\,b_2 + \frac{107597}{853680}\,b_5 - 1/4\,b_4 c_{54}$$

$$M(2,6) = \frac{814093}{37476864}\,b_3 - \frac{43503341}{666745344}\,b_4 + \frac{31559899}{819532800}\,b_5 + \frac{1206727949}{84907699200}\,b_1 - \frac{975120617049114348940031812981989566268 29}{884672469139346171238321543805472569512960}\,b_2 + \frac{229}{60240}\,b_6 + 1/20\,b_4 c_{54}$$

$$M(3,3) = -\frac{845817599}{833431680}\,b_4 + \frac{1723969}{122929920}\,b_5 + \frac{442225}{19084032}\,b_6 + \frac{1907161}{849076992}\,b_1 + \frac{284218846883624135579839539055309681 91}{897399221738547388751524989105514410 24}\,b_2 + b_4 c_{54}$$

$$M(3,4) = \frac{30644107}{368789760}\,b_5 - \frac{1000027}{57252096}\,b_6 + \frac{6737899}{471709440}\,b_1 + \frac{111153046084790373787166750753517298163}{4486996108692736943757624945527572051 20}\,b_2 - b_4 c_{54} + \frac{410237}{385848}\,b_4$$

$$M(3,5) = -\frac{217516705}{333372672}\,b_4 - \frac{741209}{12722688}\,b_6 - \frac{18285821}{4245384960}\,b_1 - \frac{516910481984296102698102049078836679 15}{1794798443477094777503049978211028820 48}\,b_2 - \frac{24947}{426840}\,b_5 + 1/2\,b_4 c_{54}$$

$$M(3,6) = -\frac{217516705}{333372672}\,b_4 - \frac{741209}{12722688}\,b_6 - \frac{18285821}{4245384960}\,b_1 - \frac{516910481984296102698102049078836679 15}{1794798443477094777503049978211028820 48}\,b_2 - \frac{24947}{426840}\,b_5 + 1/2\,b_4 c_{54}$$

$$M(4,4) = \frac{23804641}{262060800}\,b_1 + \frac{120005477}{221273856}\,b_5 + \frac{110209201}{4293907200}\,b_6 + \frac{1}{180}\,b_7 + \frac{2723762065068022432074529115499254982375 97}{1216424645066600985452692122732524783080320}\,b_2 + \frac{56535361}{421614720}\,b_3 + b_4 c_{54} - \frac{4879}{5359}\,b_4$$

$$M(4,5) = -\frac{64602839}{2358547200}\,b_1 - \frac{29661733}{954201600}\,b_6 - 1/40\,b_7 - \frac{480988850897909970622794752545229036955689}{2432849290133201970905384245465049566160640}\,b_2 + \frac{9872447}{281076480}\,b_3 - \frac{173701}{640260}\,b_5 - 1/2\,b_4 c_{54} + \frac{116695}{385848}\,b_4$$

$$M(4,6) = -\frac{17803471}{4717094400}\,b_1 - \frac{314463127}{1229299200}\,b_5 + 1/20\,b_7 + \frac{1087866595956595260465193746506692249025 33}{2211681172848365428095803859513681423782400}\,b_2 - \frac{1000027}{56215296}\,b_3 - \frac{371}{90360}\,b_6 + 1/10\,b_4 c_{54} + \frac{7519}{241155}\,b_4$$

$$M(5,5) = \frac{279377095751864675729010129709828066844101}{973139716053280788362153698186019826464256}\,b_2 + \frac{137080729}{212044800}\,b_6 + 1/8\,b_7 + \frac{1}{180}\,b_8 + \frac{1723969}{187384320}\,b_3 + \frac{175324081}{21226924800}\,b_1 + \frac{232607141}{666745344}\,b_4 + \frac{671161}{1280520}\,b_5 + 1/4\,b_4 c_{54}$$

$$M(5,6) = \frac{279377095751864675729010129709828066844101}{973139716053280788362153698186019826464256}\,b_2 + \frac{137080729}{212044800}\,b_6 + 1/8\,b_7 + \frac{1}{180}\,b_8 + \frac{1723969}{187384320}\,b_3 + \frac{175324081}{21226924800}\,b_1 + \frac{232607141}{666745344}\,b_4 + \frac{671161}{1280520}\,b_5 + 1/4\,b_4 c_{54}$$

$$M(6,6) = \frac{88445}{37476864}\,b_3 + \frac{19}{20}\,b_7 + 1/8\,b_8 + \frac{1}{180}\,b_9 + \frac{8530288801}{83343168000}\,b_4 + \frac{7090416137388876130062177660070603397759 87}{2211681172848365428095803859513681423782400 0}\,b_2 + \frac{13315201}{84907699200}\,b_1 + \frac{1260357529}{1365888000}\,b_5 + \frac{94793}{180720}\,b_6 + \frac{1}{100}\,b_4 c_{54}$$

Internal stencil

$M(j,j-3) = 1/40\, b_{j-1} + 1/40\, b_{j-2} - \frac{11}{360}\, b_j - \frac{11}{360}\, b_{j-3}$

$M(j,j-2) = 1/20\, b_{j+1} - 3/10\, b_{j-1} + 1/20\, b_{j-3} + \frac{7}{40}\, b_j + \frac{7}{40}\, b_{j-2}$

$M(j,j-1) = -3/10\, b_{j+1} - 1/40\, b_{j+2} - 3/10\, b_{j-2} - 1/40\, b_{j-3} - \frac{17}{40}\, b_j - \frac{17}{40}\, b_{j-1}$

$M(j,j) = \frac{19}{20}\, b_{j+1} + 1/8\, b_{j+2} + \frac{1}{180}\, b_{j+3} + \frac{19}{20}\, b_{j-1} + 1/8\, b_{j-2} + \frac{1}{180}\, b_{j-3} + \frac{101}{180}\, b_j$

$M(j,j+1) = -3/10\, b_{j+2} - 1/40\, b_{j+3} - 3/10\, b_{j-1} - 1/40\, b_{j-2} - \frac{17}{40}\, b_j - \frac{17}{40}\, b_{j+1}$

$M(j,j+2) = -3/10\, b_{j+1} + 1/20\, b_{j+3} + 1/20\, b_{j-1} + \frac{7}{40}\, b_j + \frac{7}{40}\, b_{j+2}$

$M(j,j+3) = 1/40\, b_{j+1} + 1/40\, b_{j+2} - \frac{11}{360}\, b_j - \frac{11}{360}\, b_{j+3}$

For the $D_2^{(8,4,6)}(B)$ operator, we give the form of the various matrices for the operator presented in the paper. As noted, to get a solution we specify the free parameters of the first derivative, $\theta_{27} = -\frac{17001835}{14684544}$, $\theta_{68} = \frac{324}{4213}$, and $\theta_{78} = \frac{441}{607}$. For the $\tilde{D}_5^{(2,1,:)}$ we have the upper portion and internal stencils given as:

- $\tilde{D}_{5,6}^{(2,1,:)}(1:5, 1:9) = (-\frac{1}{4}, 1, -\frac{3}{2}, 1, 0, -1, \frac{3}{2}, \frac{1}{4})$
- $\tilde{D}_{5,6}^{(2,1,:)}(6, 1:10) = (0, -\frac{1}{4}, 1, -\frac{3}{2}, 1, 0, -1, \frac{3}{2}, \frac{1}{4})$
- $\tilde{D}_{5,6}^{(2,1,:)}(7, 1:11) = (0, 0, -\frac{1}{4}, 1, -\frac{3}{2}, 1, 0, -1, \frac{3}{2}, \frac{1}{4})$
- $\tilde{D}_{5,6}^{(2,1,:)}(7, 1:11) = (-.233733, 0.927044, -1.629026, 2.408228, -3.696047, 3.923674, -2.159058, 0.435713, 0.033912, -0.107020, -0.158569, 0.001579)$,
- $\tilde{D}_{5,6}^{(2,1,:)}(j, j-4:j+4) = (-\frac{1}{4}, 1, -\frac{3}{2}, 1, 0, -1, \frac{3}{2}, \frac{1}{4})$

The bottom $2p$ entries are the negative of the permutation of the rows and columns of the upper $2p$ rows while $C_5^{(6)} = \text{diag}(0,0,0,0,0,0,0,118.87949,1,\ldots,1,118.87949,0,0,0,0,0,0,0)$.

For $\tilde{D}_{6,6}^{(2,1,:)}$ we have the upper portion and internal stencils given as:

- $\tilde{D}_{6,6}^{(2,1,:)}(1-8, 1:9) = \left(\frac{3}{10}, -\frac{7}{5}, \frac{12}{5}, -\frac{9}{5}, 1, -\frac{9}{5}, \frac{12}{5}, -\frac{7}{5}, \frac{3}{10}\right)$
- $\tilde{D}_{6,6}^{(2,1,:)}(j, j-4:j+4) = \left(\frac{3}{10}, -\frac{7}{5}, \frac{12}{5}, -\frac{9}{5}, 1, -\frac{9}{5}, \frac{12}{5}, -\frac{7}{5}, \frac{3}{10}\right)$

The bottom $2p$ entries are the permutation of the rows and columns of the upper $2p$ rows.

For $\tilde{D}_{7,6}^{(2,1,:)}$ we have the upper portion and internal stencils given as:

- $\tilde{D}_{7,6}^{(2,1,:)}(1-8, 1:9) = \left(-\frac{1}{2}, 3, -7, 7, 0, -7, 7, -3, \frac{1}{2}\right)$
- $\tilde{D}_{7,6}^{(2,1,:)}(j, j-4:j+4) = \left(-\frac{1}{2}, 3, -7, 7, 0, -7, 7, -3, \frac{1}{2}\right)$

The bottom $2p$ entries are the negative of the permutation of the rows and columns of the upper $2p$ rows.

For $\tilde{D}_{8,6}^{(2,1,:)}$ we have the upper portion and internal stencils given below, while the bottom $2p$ entries are the permutation of the rows and columns of the upper $2p$ rows:

- $\tilde{D}_{8,6}^{(2,1,:)}(1-8, 1:9) = (1, -8, 28, -56, 70, -56, 28, -8, 1)$
- $\tilde{D}_{8,6}^{(2,1,:)}(j, j-4:j+4) = (1, -8, 28, -56, 70, -56, 28, -8, 1)$

while $C_6^{(6)} = C_7^{(6)} = C_8^{(6)} = \text{diag}\,(0,0,,0,0,0,0,0,1,\ldots,1,0,0,0,0,0,0,0,0)$