GENERALIZED SUMMATION-BY-PARTS OPERATORS FOR THE SECOND DERIVATIVE*

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Abstract. The generalization of summation-by-parts operators for the first derivative of Del Rey Fernández et al. (J. Comput. Phys., 266, 2014) is extended to approximations of second derivatives with a constant or variable coefficient. This enables the construction of second-derivative operators with one or more of the following characteristics: i) non-repeating interior point operators, ii) nonuniform nodal distributions, and iii) exclusion of one or both boundary nodes. Definitions are proposed that give rise to generalized summation-by-parts operators that result in consistent, conservative, and stable discretizations of partial differential equations with or without mixed derivatives. It is proven that approximations to the second derivative with a variable coefficient can be constructed using the constituent matrices of the constant-coefficient operator. Moreover, for operators with a repeating interior point operator, a decomposition is proposed that makes the application of such operators particularly straightforward. A number of novel operators are constructed, including operators on the Chebyshev-Gauss quadrature nodes and operators that have a repeating interior point operator but nonuniform nodal spacing near boundaries. The various operators are compared to the application of the first-derivative operator twice in the context of the linear convection-diffusion equation with a variable coefficient.

Key words. generalized summation-by-parts, finite difference, simultaneous approximation terms, second derivative

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1. Introduction. The focus of this paper is on developing generalized summation-by-parts (GSBP) operators [7] for the second derivative with a constant or variable coefficient. In combination with simultaneous approximation terms (SATs) [3, 4, 19, 22, 24, 25] for the weak imposition of boundary conditions and inter-element coupling, GSBP operators lead to consistent, conservative, and provably stable high-order discretizations. Our first objective is to extend the classical theory of SBP operators for the second derivative in Refs. 22 and 23 and Mattsson's extension of those ideas to the approximation of the second derivative with a variable coefficient [19] to GSBP operators. Our second objective is to propose an extension and simplification of the work of Kamakoti and Pantano [16], on operators with a repeating interior point operator, to allow the straightforward inclusion of boundary nodes. This formalism leads to a very simple representation of operators with a repeating interior point operator that can be advantageous from an implementation standpoint, both for function evaluations, as well as constructing the Jacobian matrix for implicit methods.

The SBP operators in Refs. 18, 27, 29, and 8 are characterized by a uniform nodal distribution in computational space that includes both boundary nodes. We refer to these as *classical SBP operators*. The GSBP framework extends the theory of classical SBP operators to a broader class of operators characterized by one or more of the fol-

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lowing: i) non-repeating interior point operators, ii) nonuniform nodal distributions, and iii) exclusion of one or both boundary nodes. For first-derivative operators, the GSBP framework provides two advantages. First, the above generalizations can be exploited to construct operators that are more efficient than classical SBP operators while retaining the desirable properties of the SBP method [7, 21]. Second, it enables the construction of multidimensional element-type operators for the extension of SBP methods to fully unstructured grids. In this paper, we extend the GSBP framework to approximations of the second derivative.

For PDEs that contain first- and second-derivative terms, if the same first-derivative operator is used to approximate both of these terms (applied twice to approximate the second derivative), then the resultant operator approximating the second-derivative term is one order lower than the first-derivative operator. Our goal is to construct GSBP operators for the second derivative that match the order of the first derivative term and are therefore called order-matched. For stability, we will also require that they share the same norm-matrix, where first-derivative GSBP operators are constructed as $\mathsf{D}_1 = \mathsf{H}^{-1}\mathsf{Q}$, and H is called the norm-matrix. Furthermore, we are interested in operators that lead to stable semi-discrete forms for PDEs that contain mixed-derivative terms, and hence develop second-derivative operators that are compatible with the first-derivative operator used to discretize the mixed-derivative terms [19, 23]. For the constant-coefficient second derivative, the application of the first-derivative operator twice for operators with a repeating interior point operator leads to interior point operators that use information from nearly twice the number of nodes as the first-derivative operator. Alternatively, minimum-stencil operators for the second derivative can be constructed that have interior point operators that have the same stencil width as the first-derivative operator and are more efficient than the application of the first-derivative operator twice. Here we are interested in constructing approximations to the second derivative with a variable coefficient using compatible and order-matched GSBP operators with a repeating interior point operator that have minimum stencil width and exploring the potential efficiency gains of such operators.

This paper is organized as follows: in Section 2, the notation of the paper is introduced, while in Section 3 we describe the difference between element-type operators and operators with a repeating interior point operator. The first derivative is important for the construction of compatible GSBP operators for the second derivative, so a brief review is given in Section 4. General definitions for order-matched as well as compatible and order-matched GSBP operators for the second derivative are given in Section 5.1. In Section 5.2, we prove that the existence of compatible and order-matched constant-coefficient second-derivative GSBP operators guarantees the existence of compatible and order-matched variable-coefficient GSBP operators. Section 5.3 describes a useful alternative representation of GSBP operators with a repeating interior point operator, including classical SBP operators. We present two formulations for operators with a repeating interior point operator, one of which is based on the work in Refs. 22, 23, 19, 9, 10, and 8, while a more general formulation is constructed by extending the ideas of Kamakoti and Pantano [16] to include nodes at and near boundaries. The construction of various GSBP and classical SBP operators for the second derivative is discussed in Section 6, including novel GSBP operators on the Chebyshev-Gauss quadrature nodes and operators that have a repeating interior point operator with variable node-spacing at boundaries—similar in spirit to those developed by Mattsson, Almquist, and Carpenter [21], but derived by considering the

nodal distributions of the quadrature rules proposed by Alpert [1]. These operators are then validated numerically by solving the linear convection-diffusion equation with a variable coefficient in Section 7. Finally, conclusions and future work are discussed in Section 8.

2. Notation. The conventions in this paper are based on those laid out in Refs. 15, 8, and 7. Vectors are denoted with small bold letters, for example $\mathbf{x} = [x_1, \ldots, x_N]^{\mathrm{T}}$, while matrices are presented using capital letters with sans-serif font, for example M. Capital letters with script type are used to denote continuous functions on a specified domain $x \in [x_{\mathrm{L}}, x_{\mathrm{R}}]$. As an example, $\mathcal{U}(x) \in C^{\infty}[x_{\mathrm{L}}, x_{\mathrm{R}}]$ denotes an infinitely differentiable function on the domain $x \in [x_{\mathrm{L}}, x_{\mathrm{R}}]$. Lower case bold fonts are used to denote the restriction of such functions onto a grid; for example, the restriction of $\mathcal{U}$ onto the grid $\mathbf{x}$ is given by:

$$\mathbf{u} = \left[\mathcal{U}(x_1), \ldots, \mathcal{U}(x_N)\right]^{\mathrm{T}}. \tag{2.1}$$

Vectors with a subscript h, for example $\mathbf{u}_h \in \mathbb{R}^{N\times 1}$, represent the solution to a system of discrete or semi-discrete equations.

The restriction of monomials onto a set of nodes is used throughout this paper and is represented by $\mathbf{x}^j = \left[x_1^j, \ldots, x_N^j\right]^{\mathrm{T}}$, with the convention that $\mathbf{x}^j = 0$ if $j < 0$. A subscript is used to denote which derivative is being approximated; for example, D_1 denotes an SBP approximation to the first derivative. The second derivative can be approximated by applying an SBP operator approximating the first derivative twice or by constructing SBP operators that have preferential properties. For the latter, it is necessary to differentiate between approximations of the constant-coefficient derivative and the variable-coefficient derivative. The convention used is best shown through an example: D_2 represents an SBP approximation to the constant-coefficient second derivative, while $\mathsf{D}_2\left(\mathsf{B}\right)$ represents the approximation to the second derivative $\frac{\partial}{\partial x}\left(\mathcal{B}\frac{\partial \mathcal{U}}{\partial x}\right)$, where $\mathcal{B}$ is the variable coefficient, and $\mathsf{B} = \mathrm{diag}[\mathcal{B}(x_1), \ldots, \mathcal{B}(x_N)]$. We discuss the degree of SBP operators, that is, the degree of monomial for which they are exact, as well as the order of the operator. The approximation of the derivative has a leading truncation error term for each node, proportional to some power of the mesh spacing h. The order of the operator is taken as the smallest exponent of h in these truncation errors. The relation between the two for an operator approximating the m^{th} derivative is

$$\text{order} = \text{degree} - m + 1. \tag{2.2}$$

For GSBP operators with a repeating interior point operator, as well as classical SBP operators, we will discuss operators approximating higher derivatives. For example, $\mathsf{D}_{i,e}$ denotes an operator for the i^{th} derivative; if used, the subscript e differentiates among various versions of the operator.

For later use, the L_2 inner product and norm are defined as

$$(\mathcal{U}, \mathcal{V}) = \int_{x_{\mathrm{L}}}^{x_{\mathrm{R}}} \mathcal{U}\mathcal{V}\mathrm{d}x, \quad ||\mathcal{U}||^2 = \int_{x_{\mathrm{L}}}^{x_{\mathrm{R}}} \mathcal{U}^2\mathrm{d}x. \tag{2.3}$$

A discrete inner product and norm have the form

$$(\mathbf{u}, \mathbf{v})_{\mathsf{H}} = \mathbf{u}^{\mathrm{T}}\mathsf{H}\mathbf{v}, \quad ||\mathbf{u}||_{\mathsf{H}}^2 = \mathbf{u}^{\mathrm{T}}\mathsf{H}\mathbf{u}, \tag{2.4}$$

where H must be symmetric and positive definite.

3. Element-type operators and operators with a repeating interior point operator. In this paper, we develop element-type operators and operators with a repeating interior point operator that can be applied either as blocks or as elements. Consider the following four-node element-type GSBP operator for the second derivative on $x \in [-1, 1]$, constructed by applying the first derivative operator twice:

$$\mathsf{D}_2 = \begin{bmatrix} 5 & -\frac{5}{4} - \frac{15\sqrt{5}}{4} & -\frac{5}{4} + \frac{15\sqrt{5}}{4} & -\frac{5}{2} \\ \frac{3}{4}\sqrt{5} + \frac{5}{4} & -5 & \frac{5}{2} & \frac{5}{4} - \frac{3}{4}\sqrt{5} \\ \frac{5}{4} - \frac{3}{4}\sqrt{5} & \frac{5}{2} & -5 & \frac{3}{4}\sqrt{5} + \frac{5}{4} \\ -\frac{5}{2} & -\frac{5}{4} + \frac{15\sqrt{5}}{4} & -\frac{5}{4} - \frac{15\sqrt{5}}{4} & 5 \end{bmatrix}, \tag{3.1}$$

which is of order two and approximates the second derivative on the Legendre-Gauss-Lobatto nodes given by

$$\mathbf{x} = \begin{bmatrix} -1 & -\frac{1}{5}\sqrt{5} & \frac{1}{5}\sqrt{5} & 1 \end{bmatrix}^{\mathrm{T}}. \tag{3.2}$$

On a mesh with m equally sized elements on the domain $x \in [-1, 1]$, the operator becomes (ignoring the inter-element coupling for now):

$$m^2 \begin{bmatrix} \mathsf{D}_2 & & \\ & \ddots & \\ & & \mathsf{D}_2 \end{bmatrix}. \tag{3.3}$$

Mesh refinement is accomplished by increasing the number of elements. We refer to this as the *element approach*.

In contrast, consider the first-order classical SBP operator applied at N nodes on the domain $x \in [-1, 1]$, which is given as

$$\mathsf{D}_2 = \frac{(N-1)^2}{4} \begin{bmatrix} 1 & -2 & 1 & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & 1 & -2 & 1 \end{bmatrix}. \tag{3.4}$$

The operator (3.4) has a repeating interior point operator

$$\frac{1}{h^2} \begin{bmatrix} 1 & -2 & 1 \end{bmatrix}, \tag{3.5}$$

where in this case the mesh spacing is $h = \frac{2}{N-1}$. Implemented in this way, mesh refinement is carried out by increasing the number of nodes at which the interior point operator is applied. We refer to such a mesh refinement strategy as the *traditional finite-difference approach*. Alternatively, we can apply, for example, a four node operator

$$\mathsf{D}_2 = \frac{9}{4} \begin{bmatrix} 1 & -2 & 1 & \\ 1 & -2 & 1 & \\ & 1 & -2 & 1 \\ & 1 & -2 & 1 \end{bmatrix}. \tag{3.6}$$

in the same way as in (3.3), i.e., the element approach. However, the operator given in (3.1) can only be applied using the element approach.

4. Generalized SBP operators for the first derivative. The set of PDEs of interest here contain both first and second derivatives, and may or may not contain mixed derivatives. For such PDEs, just as for classical SBP methods [8, 18, 27, 29], it is possible to construct GSBP operators that lead to stable schemes if certain relationships exist between the first- and second-derivative operators. Therefore, in this section, GSBP operators for the first derivative are briefly reviewed.

To motivate the definition of an SBP operator for the first derivative, consider the linear convection equation

$$\frac{\partial \mathcal{U}}{\partial t} = -\frac{\partial \mathcal{U}}{\partial x},\ x \in [x_{\mathrm{L}}, x_{\mathrm{R}}],\ t \geq 0, \tag{4.1}$$

where specification of the initial condition and boundary conditions is not important for the present discussion. The energy method is applied to (4.1) to construct an estimate on the solution, called an energy estimate, which is then used to determine stability (for more information see Refs. 13, 14, and 17). This consists of multiplying the PDE by the solution and integrating in space and transforming the integral on the right-hand side using integration-by-parts. This leads to

$$\frac{\partial \left\|\mathcal{U}\right\|^2}{\partial t} = -\left.\mathcal{U}^2\right|_{x_{\mathrm{L}}}^{x_{\mathrm{R}}}. \tag{4.2}$$

SBP operators for the first derivative are constructed such that when the energy method is applied to the semi-discrete or fully-discrete equations, the result is analogous to (4.2). This leads to the following definition [7]

Definition 4.1. **Generalized summation-by-parts operator:** *A matrix operator $\mathsf{D}_1 \in \mathbb{R}^{N\times N}$ of degree p is an approximation to the first derivative, on the nodal distribution $\mathbf{x}$ that need neither be uniform nor include nodes on the boundaries and may have nodes that lay outside of the domain of the element $x \in [x_{\mathrm{L}}, x_{\mathrm{R}}]$, with the SBP property if*

1. $\mathsf{D}_1\mathbf{x}^j = \mathsf{H}^{-1}\mathsf{Q}\mathbf{x}^j = j\mathbf{x}^{j-1}$, $j \in [0, p]$;

2. H, *which is referred to as the norm matrix, is symmetric positive definite; and*

3. $\mathsf{Q} + \mathsf{Q}^{\mathrm{T}} = \mathsf{E}$, *where* $\left(\mathbf{x}^i\right)^{\mathrm{T}} \mathsf{E}\mathbf{x}^j = x_{\mathrm{R}}^{i+j} - x_{\mathrm{L}}^{i+j}$, $i, j \in [0, r]$, $r \geq p$.

Both classical SBP and GSBP operators can be constructed with either a diagonal-norm H or a dense-norm H, where dense norm refers to any H that is not diagonal. The matrix E is constructed as [7]

$$\mathsf{E} = \mathbf{t}_{x_{\mathrm{R}}}\mathbf{t}_{x_{\mathrm{R}}}^{\mathrm{T}} - \mathbf{t}_{x_{\mathrm{L}}}\mathbf{t}_{x_{\mathrm{L}}}^{\mathrm{T}} = \mathsf{E}_{x_{\mathrm{R}}} - \mathsf{E}_{x_{\mathrm{L}}}. \tag{4.3}$$

The vectors $\mathbf{t}_{x_{\mathrm{R}}}$ and $\mathbf{t}_{x_{\mathrm{L}}}$ satisfy the relations

$$\mathbf{t}_{x_{\mathrm{R}}}^{\mathrm{T}}\mathbf{x}^j = x_{\mathrm{R}}^j,\ \mathbf{t}_{x_{\mathrm{L}}}^{\mathrm{T}}\mathbf{x}^j = x_{\mathrm{L}}^j,\ j \in [0, r]. \tag{4.4}$$

Relation (4.4) implies that $\mathbf{t}_{x_{\mathrm{R}}}^{\mathrm{T}}\mathbf{u}$ and $\mathbf{t}_{x_{\mathrm{L}}}^{\mathrm{T}}\mathbf{u}$ are degree r approximations to $\mathcal{U}(x_{\mathrm{R}})$ and $\mathcal{U}(x_{\mathrm{L}})$, respectively, and are, therefore, of order $r+1$; that is,

$$\mathbf{t}_{x_{\mathrm{R}}}^{\mathrm{T}}\mathbf{u} = \mathcal{U}(x_{\mathrm{R}}) + \mathcal{O}\left(h^{r+1}\right),\ \mathbf{t}_{x_{\mathrm{L}}}^{\mathrm{T}}\mathbf{u} = \mathcal{U}(x_{\mathrm{L}}) + \mathcal{O}\left(h^{r+1}\right), \tag{4.5}$$

where $\mathbf{u}$ is the projection of $\mathcal{U}$ onto the nodal distribution. In (4.5), h is taken as the average spacing between nodes, for operators with a repeating interior point operator, or the size of the element, i.e., $x_{\mathrm{R}} - x_{\mathrm{L}}$, for element-type operators.

The semi-discrete representation of (4.1) using GSBP operators is

$$\frac{\mathrm{d}\mathbf{u}_h}{\mathrm{d}t} = -\mathsf{D}_1\mathbf{u}_h, \tag{4.6}$$

where we ignore, for now, the numerical imposition of boundary conditions. The energy method consists of multiplying (4.6) by $\mathbf{u}_h^{\mathrm{T}}\mathsf{H}$ and adding the transpose of the product, which gives

$$\frac{\mathrm{d}\left\|\mathbf{u}_h\right\|_{\mathsf{H}}^2}{\mathrm{d}t} = -\mathbf{u}_h^{\mathrm{T}}\left[\mathsf{H}\mathsf{D}_1 + \mathsf{D}_1^{\mathrm{T}}\mathsf{H}\right]\mathbf{u}_h. \tag{4.7}$$

Using Definition (4.1) results in

$$\frac{\mathrm{d}\left\|\mathbf{u}_h\right\|_{\mathsf{H}}^2}{\mathrm{d}t} = -\mathbf{u}_h^{\mathrm{T}}\mathsf{E}\mathbf{u}_h = -\left(\tilde{u}_{x_{\mathrm{R}}}^2 - \tilde{u}_{x_{\mathrm{L}}}^2\right), \tag{4.8}$$

where $\tilde{u}_{x_{\mathrm{R}}} = \mathbf{t}_{x_{\mathrm{R}}}^{\mathrm{T}}\mathbf{u}_h$ and $\tilde{u}_{x_{\mathrm{L}}} = \mathbf{t}_{x_{\mathrm{L}}}^{\mathrm{T}}\mathbf{u}_h$, and it can be seen that (4.8) is a discrete analogue of (4.2).

5. Generalized SBP operators for the second derivative.

5.1. Preliminaries. In this section, the definition of classical SBP operators approximating the second derivative, given by Refs. 22, 23, and 19, is extended to accommodate the derivation of GSBP operators. The form we propose combines ideas from Refs. 22, 23, and 19, as well as our extension of the ideas of Kamakoti and Pantano [16] on the interior point operator of classical SBP operators (see Section 5.3). The goal is to construct operators more accurate than the application of the first-derivative operator twice that are still amenable to the energy method, that is, operators for which discrete energy estimates can be constructed.

The motivation for the form of the operators comes in part from the integration-by-parts property of the second derivative with a variable coefficient. For example, consider the variable coefficient heat equation

$$\frac{\partial\mathcal{U}}{\partial t} = \frac{\partial}{\partial x}\left(\mathcal{B}\frac{\partial\mathcal{U}}{\partial x}\right). \tag{5.1}$$

Applying the energy method to (5.1), i.e., multiplying by the solution, integrating in space, and using integration by parts, results in

$$\frac{\mathrm{d}\|\mathcal{U}\|^2}{\mathrm{d}t} = 2\,\mathcal{B}\mathcal{U}\frac{\partial\mathcal{U}}{\partial x}\bigg|_{x_{\mathrm{L}}}^{x_{\mathrm{R}}} - 2\int_{x_{\mathrm{L}}}^{x_{\mathrm{R}}}\frac{\partial\mathcal{U}}{\partial x}\mathcal{B}\frac{\partial\mathcal{U}}{\partial x}\mathrm{d}x. \tag{5.2}$$

The application of a first-derivative classical SBP or GSBP operator leads to semi-discrete forms mimetic of (5.2). To see this, we first note that the application of the first-derivative operator twice can be decomposed as

$$\mathsf{D}_1\mathsf{B}\mathsf{D}_1 = \mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{B}\mathsf{D}_1 + \mathsf{E}\mathsf{B}\mathsf{D}_1\right], \tag{5.3}$$

which can be derived as follows:

$$\begin{aligned}\mathsf{D}_1\mathsf{B}\mathsf{D}_1 &= \mathsf{H}^{-1}\mathsf{Q}\mathsf{B}\mathsf{D}_1 = \mathsf{H}^{-1}\left(\mathsf{E} - \mathsf{Q}^{\mathrm{T}}\right)\mathsf{B}\mathsf{D}_1 \\ &= \mathsf{H}^{-1}\left[-\mathsf{Q}^{\mathrm{T}}\mathsf{H}^{-1}\mathsf{H}\mathsf{B}\mathsf{D}_1 + \mathsf{E}\mathsf{B}\mathsf{D}_1\right] = \mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{B}\mathsf{D}_1 + \mathsf{E}\mathsf{B}\mathsf{D}_1\right],\end{aligned} \tag{5.4}$$

where we have used the property of GSBP operators that $\mathsf{Q} + \mathsf{Q}^{\mathrm{T}} = \mathsf{E}$.

The semi-discrete version of (5.1), using (5.3), is

$$\frac{\mathrm{d}\mathbf{u}_h}{\mathrm{d}t} = \mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathcal{B}\mathsf{D}_1 + \mathsf{E}\mathcal{B}\mathsf{D}_1\right]\mathbf{u}_h. \tag{5.5}$$

Applying the energy method to (5.5) gives

$$\frac{\mathrm{d}\|\mathbf{u}_h\|_{\mathsf{H}}^2}{\mathrm{d}t} = \overbrace{2\mathbf{u}_h^{\mathrm{T}}\mathsf{E}\mathcal{B}\mathsf{D}_1\mathbf{u}_h}^{\approx 2\,\mathcal{B}\mathcal{U}\frac{\partial\mathcal{U}}{\partial x}\Big|_{x_{\mathrm{L}}}^{x_{\mathrm{R}}}} - \overbrace{2\left(\mathsf{D}_1\mathbf{u}_h\right)^{\mathrm{T}}\mathsf{H}\mathcal{B}\mathsf{D}_1\mathbf{u}_h}^{\approx 2\int_{x_{\mathrm{L}}}^{x_{\mathrm{R}}}\frac{\partial\mathcal{U}}{\partial x}\mathcal{B}\frac{\partial\mathcal{U}}{\partial x}\mathrm{d}x}, \tag{5.6}$$

and we see that the application of the first-derivative operator twice is mimetic of (5.2). Our goal is to retain the ability to prove stability using the energy method, but with operators that are more accurate.

The equations that an operator must satisfy in order to approximate the second derivative with a variable coefficient, denoted the degree conditions, are based on monomials restricted onto the nodes of the grid. Given that the operator must approximate $\frac{\partial}{\partial x}\left(\mathcal{B}\frac{\partial\mathcal{U}}{\partial x}\right)$, it is necessary to determine what degree monomial to insert for $\mathcal{B}$ and $\mathcal{U}$ in constructing the degree conditions. Taking $\mathcal{B} = x^k$ and $\mathcal{U} = x^s$ and inserting into the second derivative gives

$$\frac{\partial}{\partial x}\left(x^k\frac{\partial x^s}{\partial x}\right) = s(k+s-1)x^{k+s-2}. \tag{5.7}$$

To be of order p, second-derivative operators must be of degree $p+1$ (from 2.2). This implies that all combinations of $k + s \leq p + 1$ must be satisfied. Thus, the operator must satisfy the following degree conditions:

$$\mathsf{D}_2\left(\mathrm{diag}\left(\mathbf{x}^k\right)\right)\mathbf{x}^s = s(k+s-1)\mathbf{x}^{k+s-2},\ k+s \leq p+1, \tag{5.8}$$

where $\mathrm{diag}\left(\mathbf{x}^k\right)$ is a diagonal matrix such that the i^{th} diagonal entry is the i^{th} entry of $\mathbf{x}^k$. If there are N nodes in the nodal distribution, then each combination of $k + s$ in (5.8) returns a vector of N equations.

The maximum attainable degree and order for an operator for the second derivative are given by the following lemma:

LEMMA 5.1. *An operator, $\mathsf{D}_2 \in \mathbb{R}^{N\times N}$, is at most of order $p \leq N-2$ and degree $N-1$.*

Proof. Consider the degree conditions for a constant-coefficient operator:

$$\mathsf{D}_2\mathbf{x}^k = k\left(k-1\right)\mathbf{x}^{k-2},\ k \in [0, p+1]. \tag{5.9}$$

Taking $p = N-2$, the degree conditions can be recast as

$$\mathsf{D}_2\mathsf{X} = \tilde{\mathsf{X}}, \tag{5.10}$$

where $\mathsf{X} = \left[\mathbf{x}^0, \ldots, \mathbf{x}^{N-1}\right]$ and $\tilde{\mathsf{X}} = \left[\mathbf{0}, \mathbf{0}, 2\mathbf{x}^0, \ldots, (N-1)\left(N-2\right)\mathbf{x}^{N-3}\right]$. The matrix X is the Vandermonde matrix and is invertible, where the columns of X represent a basis for $\mathbb{R}^{N\times N}$. Therefore, a unique solution exists, given as $\mathsf{D}_2 = \tilde{\mathsf{X}}\mathsf{X}^{-1}$, and by examining the range of the operator D_2, i.e., $\tilde{\mathsf{X}}$, it is clear that D_2 is of most degree $N-1$ and hence order $p = N-2$. ∎

An immediate consequence of Lemma 5.1 is the following corollary:

COROLLARY 5.2. *An operator* $\mathsf{D}_2(\mathsf{B}) \in \mathbb{R}^{N\times N}$*, approximating the second derivative with a variable coefficient, is at most of order* $p = N-2$ *and degree* $N-1$*.*

Proof. The set of equations for the constant-coefficient case is a subset of the equations for the variable-coefficient operator, and therefore, by Lemma 5.1 $\mathsf{D}_2(\mathsf{B})$ *is, at best, of order* $N-2$*.* ∎

5.2. Order-matched and compatible GSBP operators for the second derivative. For classical SBP operators, one of the drawbacks of the application of the first-derivative operator twice, of degree p, is that the interior point operator uses information from $4p+1$ nodes while minimum-stencil operators have an interior point operator that uses information from $2p+1$ nodes. For GSBP operators that can only be applied using an element approach, no such concept exists. Regardless, the application of the first-derivative operator twice results in an approximation that is of lower order than the first-derivative operator. Therefore, for PDEs that contain first and second derivative terms, if the same first-derivative operator is used to approximate both terms, the approximation to the second derivative term is one order lower than that for the first-derivative term. Thus, in general, we search for GSBP operators approximating the second derivative that use the same norm-matrix and are of the same order as a given first-derivative operator. If they exist, these operators are one order more accurate than the application of the first-derivative operator twice and are denoted order matched. These ideas lead to the following definition:

DEFINITION 5.3. **Order-matched GSBP operator for the second-derivative:** *The matrix* $\mathsf{D}_2(\mathsf{B}) \in \mathbb{R}^{N\times N}$ *is a GSBP operator approximating the second derivative,* $\frac{\partial}{\partial x}\left(\mathcal{B}\frac{\partial \mathcal{U}}{\partial x}\right)$*, of degree* $p+1$ *and order* p *that is order matched to the GSBP operator* $\mathsf{D}_1 = \mathsf{H}^{-1}\mathsf{Q}$ *of degree and order* p*, on a nodal distribution* $\mathbf{x}$*, if it satisfies the equations*

$$\mathsf{D}_2\left(diag\left(\mathbf{x}^k\right)\right)\mathbf{x}^s = s(k+s-1)\mathbf{x}^{k+s-2},\ k+s \leq p+1, \tag{5.11}$$

and is of the form

$$\mathsf{D}_2(\mathsf{B}) = \mathsf{H}^{-1}\left[-\mathsf{M}(\mathsf{B}) + \mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\right],\ \textit{where}\ \mathsf{M}(\mathsf{B}) = \sum_{i=1}^{N}\mathsf{B}(i,i)\mathsf{M}_i. \tag{5.12}$$

The matrices M_i*,* B*, and* $\mathsf{D}_{1,\mathrm{b}}$ *are* $\in \mathbb{R}^{N\times N}$*,* M_i *is symmetric positive semi-definite,* $\mathsf{B} = diag(\mathcal{B}(x_1),\ldots,\mathcal{B}(x_N))$*, and* $\mathsf{D}_{1,\mathrm{b}}$ *is an approximation to the first derivative of degree and order* $\geq p+1$*.*

If one takes B to be the identity matrix, then Definition 5.3 collapses onto that given by Mattsson and Nordström [22] for classical SBP operators—defining the relevant matrix in their definition as the sum of the M_i—where we do not specify further restrictions on the form of the M_i in order to allow for GSBP operators. The extension to the variable-coefficient case, by taking the sum of matrices multiplied by the variable coefficient, is an extension and simplification of the work by Kamakoti and Pantano [16], who decompose the interior point operator of finite-difference approximations to the second derivative with a variable coefficient as the sum of the variable coefficient multiplying a third-order tensor. Definition 5.3 can be applied to dense-norm GSBP operators, though we do not pursue this further.

Applying the energy method to Definition 5.3 leads to terms similar to those obtained using the application of the first-derivative operator twice. Consider discretizing (5.1) using a GSBP operator, as given in Definition 5.3, which results in the

following semi-discrete system:

$$\frac{\mathrm{d}\mathbf{u}_h}{\mathrm{d}t} = \mathsf{H}^{-1}\left[-\mathsf{M}\left(\mathsf{B}\right) + \mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\right]\mathbf{u}_h. \tag{5.13}$$

Applying the energy method to (5.13) results in

$$\frac{\mathrm{d}\|\mathbf{u}\|_{\mathsf{H}}^2}{\mathrm{d}t} = 2\mathbf{u}_h^{\mathrm{T}}\mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\mathbf{u}_h - 2\mathbf{u}_h^{\mathrm{T}}\mathsf{M}\left(\mathsf{B}\right)\mathbf{u}_h. \tag{5.14}$$

We see that Definition 5.3 results in the correct boundary terms and a negative semi-definite term, i.e., $-2\mathbf{u}_h^{\mathrm{T}}\mathsf{M}\left(\mathsf{B}\right)\mathbf{u}_h$, as in the continuous case (5.2). However, it is not fully mimetic of the continuous case. Nevertheless, with appropriate SATs, Definition 5.3 is sufficient to prove stability of the semi-discrete form of PDEs that do not contain mixed derivatives. Further restrictions need to be applied to Definition 5.3 such that stability can be proven for the semi-discrete form of PDEs with mixed derivatives. One possibility is referred to as compatible operators [23], which leads to the following definition:

Definition 5.4. **Compatible and order-matched GSBP operator for the second-derivative:** *A diagonal-norm order-matched GSBP operator,* $\mathsf{D}_2(\mathsf{B}) \in \mathbb{R}^{N\times N}$*, for the second derivative, is compatible with the first-derivative GSBP operator,* D_1 *of order and degree* p*, if in addition to the requirements of Definition 5.3,*

$$\mathsf{M}\left(\mathsf{B}\right) = \mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{B}\mathsf{D}_1 - \mathsf{R}\left(\mathsf{B}\right), \text{ where } \mathsf{R}\left(\mathsf{B}\right) = \sum_{i=1}^{N}\mathsf{B}(i,i)\mathsf{R}_i, \tag{5.15}$$

where the R_i *matrices are symmetric negative semi-definite, therefore,*

$$\mathsf{D}_2\left(\mathsf{B}\right) = \mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{B}\mathsf{D}_1 + \mathsf{R}\left(\mathsf{B}\right) + \mathsf{E}\mathsf{B}\mathsf{D}_{1,b}\right]. \tag{5.16}$$

The decomposition in (5.16) is inspired by the observation that the application of the first-derivative GSBP operators twice to approximate the second derivative with a variable coefficient can be reformulated as given in (5.3). The idea of constructing classical SBP approximations to the second derivative as the application of the first-derivative operator twice plus corrective terms was first proposed by Mattsson et al. [23] and later used by Mattsson [19] to construct classical SBP operators to approximate the second derivative with a variable coefficient. We say corrective terms since not only has the term $\mathsf{H}^{-1}\mathsf{R}\left(\mathsf{B}\right)$ been added, but $\mathsf{E}\mathsf{B}\mathsf{D}_1$ has been replaced by $\mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}$, which can be construed as adding a corrective term to $\mathsf{E}\mathsf{B}\mathsf{D}_1$. The definition of compatible operators is limited to diagonal-norm operators. For the variable-coefficient case, it is unclear how to prove stability using the energy method for compatible dense-norm operators (see Mattsson and Almquist [20] for a discussion and potential solution).

Applying the energy method to Definition 5.4 results in terms fully mimetic of the continuous case. Discretizing (5.1) with a GSBP operator as given by Definition 5.4 results in the following semi-discrete equations:

$$\frac{\mathrm{d}\mathbf{u}_h}{\mathrm{d}t} = \mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{B}\mathsf{D}_1 + \mathsf{R}\left(\mathsf{B}\right) + \mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\right]. \tag{5.17}$$

Applying the energy method to (5.17) results in

$$\frac{\mathrm{d}\|\mathbf{u}_h\|_{\mathsf{H}}^2}{\mathrm{d}t} = 2\mathbf{u}_h^{\mathrm{T}}\mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\mathbf{u}_h - 2\left(\mathsf{D}_1\mathbf{u}_h\right)^{\mathrm{T}}\mathsf{H}\mathsf{B}\mathsf{D}_1\mathbf{u}_h + 2\mathbf{u}_h^{\mathrm{T}}\mathsf{R}\left(\mathsf{B}\right)\mathbf{u}_h. \tag{5.18}$$

Now the right-hand side of (5.17) fully mimics the continuous case (5.2), where $2\mathbf{u}_h^{\mathrm{T}}\mathsf{R}\left(\mathsf{B}\right)\mathbf{u}_h$ adds a term of order of the discretization error.

The compatibility that is necessary is between the first-derivative operators approximating the mixed derivatives and the second-derivative operator for the same spatial direction. In addition, for an energy estimate to exist, with appropriate SATs, the norms H of all operators in the same spatial direction must be the same. In practice, this means that all first-derivative terms are typically approximated using the same GSBP operator.

Constructing the degree conditions (5.8) using the application of the first-derivative operator twice results in

$$\mathsf{D}_1\mathrm{diag}\left(\mathbf{x}^k\right)\mathsf{D}_1\mathbf{x}^s = s\mathsf{D}_1\mathbf{x}^{s+k-1} = s(s+k-1)\mathbf{x}^{s+k-2},\ s+k \leq p+1,\ s \leq p. \tag{5.19}$$

Equations (5.19) show that only the degree conditions for $s = p+1,\ k = 0$ are not satisfied by the application of the first-derivative operator twice. This observation leads to the following theorem:

THEOREM 5.5. *The existence of a diagonal-norm compatible and order-matched constant-coefficient GSBP operator* D_2 *of order* p *and degree* $p+1$ *is sufficient for the existence of a compatible and order-matched variable-coefficient GSBP operator* $\mathsf{D}_2\left(\mathsf{B}\right)$*, for* $p+1 \leq N-1$ *and* $N \geq 3$.

Proof. First, by Lemma (5.1), we must have at least three nodes to obtain an approximation of at least first order. We assume that the constant-coefficient operator exists, given as

$$\mathsf{D}_2 = \mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{D}_1 + \mathsf{R}_{\mathrm{c}} + \mathsf{E}\mathsf{D}_{1,\mathrm{b}}\right]. \tag{5.20}$$

Consider constructing the variable-coefficient operator as

$$\mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{B}\mathsf{D}_1 + \frac{\sum_{i=1}^{N} b_i}{N}\mathsf{R}_{\mathrm{c}} + \mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\right], \tag{5.21}$$

where R_{c} and $\mathsf{D}_{1,\mathrm{b}}$ are from the constant-coefficient operator. As has been argued, the additional degree conditions that must be satisfied are for $(k,s) = (0,p+1)$. Since (5.21) collapses onto the constant-coefficient operator for this condition, it automatically satisfies these additional conditions. It remains to be shown that the remaining degree conditions are still satisfied.

Now $\mathsf{D}_{1,\mathrm{b}} = \mathsf{D}_1 + \mathsf{A}$, where A is a corrective term such that $\mathsf{D}_{1,\mathrm{b}}$ is at least one order more accurate than the first-derivative operator (see Definition 5.4). Using the decomposition of the first derivative twice (5.3), (5.21) can be recast as

$$\mathsf{D}_1\mathsf{B}\mathsf{D}_1 + \mathsf{H}^{-1}\left\{\frac{\sum_{i=1}^{N} b_i}{N}\mathsf{R}_{\mathrm{c}} + \mathsf{E}\mathsf{B}\mathsf{A}\right\}. \tag{5.22}$$

Examining the constant-coefficient version of (5.21), it can be seen that both $\mathsf{A}\mathbf{x}^s$ and $\mathsf{R}_c\mathbf{x}^s$ must be be the zero vector for $\mathbf{x}^s$ for $s \leq p$. Therefore, we have proven that (5.21) leads to a compatible and order-matched GSBP operator for the second derivative with a variable coefficient. □

The implication of Theorem 5.5 is that the search for compatible and order-matched GSBP operators for the variable-coefficient case reduces to the search for compatible and order-matched GSBP operators for the constant-coefficient case. This substantially simplifies both the proof that compatible and order-matched GSBP operators exist for a given nodal distribution and the construction of such operators. The implications of this will be further discussed in Section 6.

5.3. Alternative representation of GSBP operators with a repeating interior point operator. In this section we show that operators constructed based on ideas in Refs. 22, 23, 19, 9, 10, and 8 can be reformulated into a form based on the ideas of Kamakoti and Pantano [16]. The alternative form of the operator is not only convenient for analysis, but also from an implementation standpoint, as it reduces the application of the operator to one loop. The alternative form is also advantageous for the construction of implicit methods that require the linearization of the compatible and order-matched GSBP operator, since the linearization is completely transparent. Moreover, it is a convenient formalism for presenting particular instances of operators.

For operators with a repeating interior point operator, the added corrective terms must result in an interior point operator that has the same bandwidth as the interior point operator of the first-derivative operator, that is, a centered interior point operator of order $2p$ which is a function of the solution at $2p+1$ nodes. On the interior, the corrective term $\mathsf{R}(\mathsf{B})$ is the sum of second-order approximations to even derivatives (see the supplementary material for more details). This form arises by noting that minimum-stencil centered finite-difference operators can be decomposed as the application of the first-derivative operator twice plus second-order approximations to even derivatives [23].

The first form is given as

$$\mathsf{D}_2(\mathsf{B}) = \mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{B}\mathsf{D}_1 + \mathsf{R}(\mathsf{B}) + \mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\right], \tag{5.23}$$

where

$$\mathsf{R}(\mathsf{B}) = \sum_{i=p+1}^{2p} \alpha_i^{(p)} h^{2i-1} \left(\mathsf{D}_{i,p}\right)^{\mathrm{T}} \mathsf{C}_i^{(p)} \mathsf{B}\mathsf{D}_{i,p}, \tag{5.24}$$

where $\mathsf{R}(\mathsf{B})$, $\mathsf{D}_{i,p}$, and $\mathsf{C}_i^{(p)}$ are all $N \times N$ matrices. In the supplementary material, we give more details on how to derive $\mathsf{R}(\mathsf{B})$ as well as the details of the operators used in this paper. Constructed this way, for appropriate values of the α coefficients and positive semi-definite $\mathsf{C}_i^{(p)}$ (see the supplementary material), the operators have interior point operators that are of the same bandwidth as the first-derivative operator, and the $\mathsf{R}(\mathsf{B})$ corrective term is guaranteed to be negative semi-definite, a necessary condition for an energy estimate to exist.

Following the lead of Kamakoti and Pantano [16], we can reorganize (5.23) in terms of the variable coefficient as

$$\mathsf{D}_2(\mathsf{B}) = \sum_{i=1}^{N} \mathsf{B}(i,i)\mathsf{M}_i, \tag{5.25}$$

where M_i in (5.25) are $N \times N$ matrices. Again, taking our cue from Kamakoti and Pantano [16], the second form we propose is constructed by collapsing (5.25) by retaining only the nonzero blocks from the M_i. The resulting operator applied to a vector $\mathbf{u}$, with a slight abuse of notation, can be constructed as

$$\mathsf{D}_2\left(\mathsf{B}\right)\mathbf{u} = \sum_{i=1}^{g} \mathsf{B}(i,i)\mathsf{F}_i\mathbf{u}_i + \tilde{\mathsf{F}}_i\mathbf{u}_{N-i+1} + \sum_{i=g+1}^{N-g} \mathsf{B}(i,i)\mathsf{F}_{\mathrm{INT}}\mathbf{u}_i, \tag{5.26}$$

where the $\tilde{\mathsf{F}}_i$ matrices are the permutation of the rows and columns of the F_i matrices. The $\mathbf{u}_i$ are portions of the vector $\mathbf{u}$, and $\mathsf{F}_{\mathrm{INT}}$ is a matrix that originates from the coefficients of the interior point operator. Form (5.26) is to be understood as constructing the vector $\mathsf{D}_2\left(\mathsf{B}\right)\mathbf{u}$ using the sequence implied by the right-hand side of (5.26). The transition from form (5.23) to (5.25) and finally (5.26) is best understood using a simple example.

Consider the following compatible and order-matched classical first-order second-derivative SBP operator on five nodes:

(5.27)

$$4h\mathsf{D}_2\left(\mathsf{B}\right) =$$

$$\begin{bmatrix} 10b_1-6b_2 & 8b_2-16b_1 & -2b_2+6b_1 & 0 & 0 \\ 4b_2 & 2b_1-2b_3-8b_2 & -2b_1+4b_2+2b_3 & 0 & 0 \\ -b_2+b_1 & -2b_1+4b_2+2b_3 & -3b_2-3b_4+b_1-4b_3+b_5 & 2b_3+4b_4-2b_5 & -b_4+b_5 \\ 0 & 0 & 2b_3+4b_4-2b_5 & -2b_3+2b_5-8b_4 & 4b_4 \\ 0 & 0 & -2b_4+6b_5 & 8b_4-16b_5 & -6b_4+10b_5 \end{bmatrix},$$

where we have used the short form $b_i = \mathsf{B}(i,i)$. Using form (5.25) we have

$$\mathsf{D}_2\left(\mathsf{B}\right)\mathbf{u} = \sum_{i=1}^{5} b_i\mathsf{M}_i\mathbf{u}, \tag{5.28}$$

where

$$4h^2\mathsf{M}_1 = \begin{bmatrix} 10 & -16 & 6 & 0 & 0 \\ 0 & 2 & -2 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, 4h^2\mathsf{M}_2 = \begin{bmatrix} -6 & 8 & -2 & 0 & 0 \\ 4 & -8 & 4 & 0 & 0 \\ -1 & 4 & -3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{5.29}$$

$$4h^2\mathsf{M}_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & 2 & 0 & 0 \\ 0 & 2 & -4 & 2 & 0 \\ 0 & 0 & 2 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{5.30}$$

$$4h^2\mathsf{M}_4 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -3 & 4 & -1 \\ 0 & 0 & 4 & -8 & 4 \\ 0 & 0 & -2 & 8 & -6 \end{bmatrix}, 4h^2\mathsf{M}_5 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & -2 & 2 & 0 \\ 0 & 0 & 6 & -16 & 10 \end{bmatrix}. \tag{5.31}$$

Note that M_4 and M_5 are equal to the permutation of the rows and columns of M_2 and M_1, respectively. On this five node mesh (5.26) is given by

$$\mathsf{D}_2\left(\mathsf{B}\right)\mathbf{u} = b_1\mathsf{F}_1\mathbf{u}(1:3) + b_2\mathsf{F}_2\mathbf{u}(1:3) + b_3\mathsf{F}_3\mathbf{u}(2:4) + b_4\mathsf{F}_4\mathbf{u}(3:5) + b_5\mathsf{F}_5\mathbf{u}(3:5), \tag{5.32}$$

where

$$\begin{aligned} &\mathsf{F}_1 = \mathsf{M}_1(1:3,1:3) \quad \mathsf{F}_2 = \mathsf{M}_2(1:3,1:3), \quad \mathsf{F}_3 = \mathsf{M}_3(2:4,2:4), \\ &\mathsf{F}_4 = \mathsf{M}_4(3:5,3:5), \quad \mathsf{F}_5 = \mathsf{M}_5(3:5,3:5). \end{aligned} \tag{5.33}$$

To apply (5.26) to more than five nodes only requires shifting the indices of $\mathbf{u}$ and adding more applications of F_3. Thus, for N nodes we have

$$\begin{aligned} \mathsf{D}_2\left(\mathsf{B}\right)\mathbf{u} \quad = \quad & b_1\mathsf{F}_1\mathbf{u}(1:3) + b_2\mathsf{F}_2\mathbf{u}(1:3) \\ & + b_{N-1}\mathsf{F}_4\mathbf{u}(N-2:N) + b_N\mathsf{F}_5\mathbf{u}(N-2:N) \\ & + \sum_{i=3}^{N-2} b_i\mathsf{F}_{\mathrm{INT}}\mathbf{u}(i-1:i+1), \end{aligned} \tag{5.34}$$

where $\mathsf{F}_{\mathrm{INT}} = \mathsf{F}_3$.

Form (5.26) demonstrates that the increased computational expense between a finer mesh and a coarse mesh originates from the increased application of $\mathsf{F}_{\mathrm{INT}}$. Table 1 delineates the number of nonzero elements in $\mathsf{F}_{\mathrm{INT}}$ that result for $p \in [1,4]$ and we find that for $p \leq 3$ the number of floating point operations to implement the interior point operator is greater for the compatible and order-matched operators, as compared to the application of the first-derivative operator twice, even though the stencil size is the same. This contrasts with the constant-coefficient case, where the resultant operator not only has a smaller interior stencil, but the number of floating point operations required to build the interior point operator is $2p+1$ as compared to $4p+1$ required to build the interior point operator from the application of the first-derivative operator twice. We remark that for the constant-coefficient operator it is more efficient to add the various matrices in (5.23) once and for all and apply the operator point-wise.

6. Construction of GSBP operators for the second derivative.

6.1. Preliminaries. For compatible order-matched GSBP operators it is necessary to first solve for the first-derivative GSBP operator, the degree conditions for which are given by

$$\mathsf{Q}\mathbf{x}^j = j\mathsf{H}\mathbf{x}^{j-1}, \quad j \in [0,p]. \tag{6.1}$$

TABLE 1
The number of nonzero entries in F_{INT}

p	$\mathsf{D}_2(\mathsf{B})$	$\mathsf{D}_1\mathsf{B}\mathsf{D}_1$
1	7	4
2	19	16
3	37	36
4	61	64
p	$(2p+1)+2\sum_{i=1}^{p} p+i$	$4p^2$

The solution to the degree conditions (5.8) and (6.1) typically results in free parameters that must be specified. This naturally leads to the concept of optimization. Here we use the discrete GSBP L_2 inner product of the error as the objective function to be minimized. For the first-derivative operator, D_1 of order p, we obtain

$$J_{p+1} = \mathbf{e}_{p+1}^{\mathrm{T}} \mathsf{H} \mathbf{e}_{p+1}, \tag{6.2}$$

where the error vector is

$$\mathbf{e}_{p+1} = \mathsf{D}_1 \mathbf{x}^{p+1} - (p+1)\,\mathbf{x}^{p}. \tag{6.3}$$

For GSBP operators approximating the second derivative with a variable coefficient, there are several error vectors, each of which is given by

$$\mathbf{e}_{k,s} = \mathsf{D}_2 \left(\operatorname{diag}\left(\mathbf{x}^k\right)\right) \mathbf{x}^s - s(s+k-1)\mathbf{x}^{s+k-2},\ k+s=p+2 \tag{6.4}$$

and the objective function is constructed as

$$J_{p+2} = \sum_{i=0}^{p+2} \left(\mathbf{e}_{i,p+2-i}\right)^{\mathrm{T}} \mathsf{H} \mathbf{e}_{i,p+2-i}. \tag{6.5}$$

6.2. Operators with a repeating interior point operator: Classical SBP and hybrid Gauss-trapezoidal operators. In addition to classical SBP operators on uniform grids, we also examine operators with a repeating interior point operator that have a number of nodes near the boundaries that are not equally spaced. This idea was first proposed by Mattsson et al. [21]. These operators have some very attractive properties. By allowing the nodal spacing to vary near the boundaries, it is possible to reduce the magnitude of the error originating from the point operators near and at boundary nodes [21]. For diagonal-norm classical SBP operators this is particularly beneficial, as the order of the operator reduces by half at these nodes. The construction of these operators follows the same steps as for classical SBP operators and so we use form (5.23).

Deriving the optimal nodal locations beyond two or three nodes while at the same time ensuring that a positive-definite norm matrix can be found is difficult [21]. Alternatively, Del Rey Fernández et al. [7] have proven that the norm matrix of a GSBP operator is associated with a quadrature rule of certain degree. Thus, if quadrature rules with the desired properties exist, then those nodal locations can be used to construct GSBP operators. It turns out that Alpert [1] proposed such quadrature rules guaranteed to have positive weights up to degree twenty. The nodal

locations and quadrature weights are determined from the solution to

$$\sum_{i=1}^{j} \tilde{w}_i \tilde{x}_i^r = \frac{B_{r+1}(a)}{r+1}, \quad r = 0, 1, \ldots, 2j-2, \tag{6.6}$$

where $B_i(x)$ is the i^{th} Bernoulli polynomial, and $B_0(x) = 1$, and the parameters a and j are chosen so that a particular degree is attained. If they are chosen such that $a = j$, which is the approach taken here, then it is possible to show that the resultant quadrature rule has positive weights up to degree twenty [1]. To enforce a node at the left boundary the equations (6.6) are constrained by

$$\tilde{x}_1 = 0. \tag{6.7}$$

Since the resultant nodal distribution is symmetric it thus includes both boundary nodes. We consider two nodal distributions: 1) hybrid Gauss-trapezoidal (HGT), which does not include the boundary nodes, and 2) hybrid Gauss-trapezoidal-Lobatto (HGTL), which does include the boundary nodes. To construct a nodal distribution on $x \in [0, 1]$ and quadrature weights, the following relations are used:

$$\begin{aligned} &x_i = h\tilde{x}_i, \quad x_{n-(i-1)} = 1 - h\tilde{x}_i, \quad i \in [1, j], \\ &x_{i+j+1} = h(a+i), \quad i \in [0, n-1], \\ &\omega_i = h\tilde{\omega}_i \ \forall i \in [1, j] \text{ and } \omega_i = h \text{ for the remaining } i, \end{aligned} \tag{6.8}$$

where $h = \frac{1}{n+2a-1}$, n is the number of uniformly distributed nodes, the total number of nodes is given as $N = n + 2j$, and ω_i are the quadrature weights, i.e.

$$\int_{x_{\text{L}}}^{x_{\text{R}}} f \mathrm{d}x \approx \sum_{i=1}^{j} \left(f(x_i) + f(x_{N-i+1}) \right) \omega_i + \sum_{i=j+1}^{N-j} f(x_i) h. \tag{6.9}$$

Rather than using the quadrature rules given by Alpert [1], we use only his nodal distributions. This is done to allow variation in the quadrature weights at the first $2p$ nodes which contain some of the equally spaced nodes; otherwise, we can only construct element-type operators using the H norm matrix that results from Alpert's quadrature rules. Thus, the resultant norm matrix H and associated quadrature rules, which are different from those given by Alpert [1], naturally result from the solution to the degree conditions.

We summarize the steps taken to construct both classical SBP operators and the hybrid Gauss-trapezoidal-Lobatto and hybrid Gauss-trapezoidal operators:

- solve the degree conditions (6.1) for the first-derivative GSBP operator;
- minimize J_{p+1} (6.2) if there are free parameters;
- set any remaining free parameters to zero;
- construct the GSBP operator for the second derivative using (5.23);
- form and solve the first $2p$ degree conditions (5.8);
- choose a family of operators and specify free parameters through optimization, using the objective function (6.5), with the constraint that the $\mathsf{C}_i^{(p)}$ matrices in (5.24) are positive semi-definite; and then
- set any remaining free parameters to zero.

The form (5.23) leads to nonlinear degree conditions and hence multiple families of solutions. Each one of these families can be optimized with the constraint that the $\mathsf{C}_i^{(p)}$ matrices are positive semi-definite. Some of these families are more difficult to optimize than others, in particular for hybrid Gauss-trapezoidal-Lobatto and hybrid Gauss-trapezoidal operators. Here we choose one family for each operator that is easily optimized by Maple© for operators of orders two and three. However, for order four hybrid Gauss-trapezoidal-Lobatto and hybrid Gauss-trapezoidal operators we had significant difficulty solving the degree conditions and had to resort to manually zeroing the undetermined coefficients and the general solution to the degree conditions for these operators is still an open question.

6.3. Diagonal-norm GSBP operators on Gauss quadrature nodal distributions. We construct a number of diagonal-norm GSBP operators on Gauss quadrature nodal distributions. Definition 5.4 requires the construction of $\mathsf{R}(\mathsf{B})$. In the most general case, $\mathsf{R}(\mathsf{B})$ can be constructed as

$$\mathsf{R}(\mathsf{B}) = \sum_{i=1}^{N} \mathsf{B}(i,i)\mathsf{R}_i, \tag{6.10}$$

with the restriction that R_i is symmetric negative semi-definite for all i. This formulation leads to linear degree conditions (5.8), but nonlinear constraints for R_i to be symmetric negative semi-definite. Alternatively, R_i is constructed to be symmetric negative semi-definite as follows:

$$\mathsf{R}_i = -\mathsf{L}_i^{\mathrm{T}} \mathsf{\Lambda}_i \mathsf{L}_i, \tag{6.11}$$

where L_i is lower unitriangular and $\mathsf{\Lambda}_i$ is a diagonal matrix. Now the constraint that R_i be symmetric negative semi-definite reduces to the constraint that $\mathsf{\Lambda}_i$ be positive semi-definite; however, the degree conditions become nonlinear. Although (6.11) is guaranteed to result in compatible order-matched operators, if solutions can be found, the resultant system of equations is very difficult to solve, particularly for operators with many nodes. This motivates the search for simplifications of $\mathsf{R}(\mathsf{B})$, as have been found for classical SBP operators (see the supplementary material).

Rather than the above, we seek a construction of $\mathsf{R}(\mathsf{B})$ such that it is of the form (6.10) and satisfies the requirement that R_i be symmetric negative semi-definite, but does not require the solution of a large system of nonlinear equations. We do this by taking advantage of Theorem 5.5. We first solve for the constant-coefficient compatible and order-matched GSBP operator for the second derivative, given by

$$\mathsf{D}_2 = \mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{D}_1 + \mathsf{R}_{\mathrm{c}} + \mathsf{E}\mathsf{D}_{1,\mathrm{b}}\right], \tag{6.12}$$

which has degree conditions

$$\mathsf{D}_2\mathbf{x}^k = k(k-1)\mathbf{x}^{k-2}, \quad j \in [0, p+1]. \tag{6.13}$$

By Theorem 5.5, if R_{c} is symmetric negative semi-definite, then a compatible and order-matched GSBP operator is given by

$$\mathsf{D}_2(\mathsf{B}) = \mathsf{H}^{-1}\left[-\mathsf{D}_1^{\mathrm{T}}\mathsf{H}\mathsf{B}\mathsf{D}_1 + \sum_{i=1}^{N} \frac{\mathsf{B}(i,i)}{N}\mathsf{R}_{\mathrm{c}} + \mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\right]. \tag{6.14}$$

The general steps to construct compatible and order-matched GSBP operators, given a nodal distribution $\mathbf{x}$, are as follows:

- solve the degree conditions (6.1) for the first-derivative GSBP operator;
- minimize J_{p+1} (6.2) if there are free parameters;
- set any remaining free parameters to zero;
- solve the degree conditions for the constant-coefficient second derivative (6.13);
- use free parameters to ensure that R_c is negative semi-definite; and then
- optimize using J_{p+2} (6.5) and set any remaining free parameters to zero.

As examples, we have constructed element-type operators on the Chebyshev-Gauss quadrature nodes defined by

$$x_k = -\cos\left(\frac{(2k+1)\,\pi}{2\,(N-1)+2}\right), \quad k \in [0, N-1] \tag{6.15}$$

Even though the first-derivative GSBP operators are constructed on the Chebyshev-Gauss quadrature nodes, the operators that are obtained are not the classical pseudo-spectral difference operators associated with that nodal distribution, which have dense norms [26].

As a point of comparison, we construct operators on the Legendre-Gauss-Lobatto quadrature nodes, for which the resulting pseudo-spectral difference operators have been shown to be diagonal-norm GSBP operators [11]. The nodal distribution, for N nodes, is given by the solution to

$$\frac{\mathrm{d}P_{N-1}}{\mathrm{d}x} = 0, \tag{6.16}$$

where the Legendre polynomial, P_N, has the explicit representation

$$P_{N-1} = \frac{1}{2^N}\sum_{k=0}^{N}\binom{N}{k}^2 (x-1)^{N-k}\,(x+1)^k\,. \tag{6.17}$$

6.4. Summary of operators. Table 2 lists the abbreviations used to refer to the GSBP operators studied in Section 7. The arguments of the abbreviations can take the following values:

- F^2 for the application of the first-derivative operator twice or CO for compatible and order-matched operators
- *elem* denotes that the operator is applied using the element approach, while *trad* is an operator applied using the traditional finite-difference approach
- N is the number of nodes in each element (not applicable to operators applied using the traditional finite-difference approach)
- p is the order of the second-derivative operator

The operators used in this paper are available electronically, and their description is given in the supplementary material. The degree and order of operators as the application of the first-derivative operator twice, on the Chebyshev-Gauss quadrature node with N nodes, are given as

$$\text{degree} = \lceil \tfrac{N}{2} \rceil, \text{ and } \quad \text{order} = \lceil \tfrac{N}{2} \rceil - 1, \tag{6.18}$$

where $\lceil \cdot \rceil$ is the ceiling operator which returns the closest integer greater than or equal to the argument. For compatible and order-matched operators on these nodal distributions, the relationship is given as

$$\text{degree} = \lceil \tfrac{N}{2} \rceil + 1, \text{ and } \quad \text{order} = \lceil \tfrac{N}{2} \rceil. \tag{6.19}$$

TABLE 2
Abbreviations for GSBP operators[1]

Abbreviation	Operator
$\mathrm{LGL}(\mathrm{F}^2, \mathrm{elem}, N, p)$	Diagonal-norm element-type GSBP operators constructed on the Legendre-Gauss-Lobatto quadrature nodes.
$\mathrm{CG}(\mathrm{F}^2 \text{ or } \mathrm{CO}, \mathrm{elem}, N, p)$	Diagonal-norm element-type GSBP operators constructed on the Chebyshev-Gauss quadrature nodes.
$\mathrm{CSBP}(\mathrm{F}^2 \text{ or } \mathrm{CO}, \mathrm{elem} \text{ or } \mathrm{trad}, N, p)$	Diagonal-norm classical SBP operator with a repeating interior point operator.
$\mathrm{HGTL}(\mathrm{F}^2 \text{ or } \mathrm{CO}, \mathrm{elem} \text{ or } \mathrm{trad}, N, p)$	Diagonal-norm GSBP operators on the hybrid Gauss-trapezoidal-Lobatto nodal distribution with a repeating interior point operator.
$\mathrm{HGT}(\mathrm{F}^2 \text{ or } \mathrm{CO}, \mathrm{elem} \text{ or } \mathrm{trad}, N, p)$	Diagonal-norm GSBP operator on the hybrid Gauss-trapezoidal nodal distribution with a repeating interior point operator.

On the Legendre-Gauss-Lobatto quadrature nodes, with N nodes, the first-derivative operator is of degree $N-1$. This means that the application of the first-derivative operator is of degree $N-1$ and is therefore of maximum degree as per Lemma (5.2). We therefore cannot construct compatible and order-matched operators on this nodal distribution.

Finally, for operators with a repeating interior point operator, the following relations hold for the application of the first-derivative operator twice, of order p:

$$\text{degree} = p, \text{ and } \quad \text{order} = p - 1, \tag{6.20}$$

while for order-matched operators, the relationship is given as

$$\text{degree} = p + 1, \text{ and } \quad \text{order} = p. \tag{6.21}$$

7. Numerical results. In this section, various GSBP operators are characterized in the context of the steady linear convection-diffusion equation given as

$$-a\frac{\partial \mathcal{U}}{\partial x} + \mu \frac{\partial}{\partial x}\left(\mathcal{B}\frac{\partial \mathcal{U}}{\partial x}\right) + \mathcal{S} = 0, \; x \in [x_{\mathrm{L}}, x_{\mathrm{R}}], \; \mathcal{B} > 0, \tag{7.1}$$

with boundary conditions

$$\alpha_{x_{\mathrm{L}}}\mathcal{U}_{x_{\mathrm{L}}} + \beta_{x_{\mathrm{L}}}\mathcal{B}_{x_{\mathrm{L}}} \left.\frac{\partial \mathcal{U}}{\partial x}\right|_{x_{\mathrm{L}}} = \mathcal{G}_{x_{\mathrm{L}}} \text{ and } \alpha_{x_{\mathrm{R}}}\mathcal{U}_{x_{\mathrm{R}}} + \beta_{x_{\mathrm{R}}}\mathcal{B}_{x_{\mathrm{R}}} \left.\frac{\partial \mathcal{U}}{\partial x}\right|_{x_{\mathrm{R}}} = \mathcal{G}_{x_{\mathrm{R}}}. \tag{7.2}$$

[1]The parameter N is only relevant to operators applied using the element approach.

We solve (7.1), subject to (7.2) with a variable coefficient given by

$$\mathcal{B} = 2 + \sin(10x), \tag{7.3}$$

We set $a = 1$ and $\mu = \frac{1}{10}$ and solve on the domain $x \in \left[\frac{32}{100}, \frac{94}{100}\right]$, while the source term $\mathcal{S}$ and the functions $\mathcal{G}_{x_\mathrm{L}}$ and $\mathcal{G}_{x_\mathrm{R}}$ are chosen such that the solution to (7.1) and (7.2) is

$$\mathcal{U}(x) = \exp\left(\frac{a}{\mu}\left(\frac{\tan^{-1}\left(\frac{2\tan(5x)+1}{\sqrt{3}}\right)}{5\sqrt{3}}\right)\right). \tag{7.4}$$

The discrete equations for a single block or element are given as

$$\begin{aligned} &-a\mathsf{D}_1\mathbf{u}_h + \mu\mathsf{H}^{-1}\left[-\mathsf{D}_1^\mathrm{T}\mathsf{H}\mathsf{B}\mathsf{D}_1 + \mathsf{R}(\mathsf{B}) + \mathsf{E}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\right]\mathbf{u}_h \\ &+\mathbf{SAT}_{x_\mathrm{L}} + \mathbf{SAT}_{x_\mathrm{R}} + \mathbf{s} = 0, \end{aligned} \tag{7.5}$$

where the additional two terms are the SATs to impose the boundary conditions. The SATs are constructed to mimic the continuous boundary conditions (7.2) and have the form

$$\begin{aligned} \mathbf{SAT}_{x_\mathrm{L}} &= \sigma_{x_\mathrm{L}}\mathsf{H}^{-1}\mathsf{E}_{x_\mathrm{L}}\left(\alpha_{x_\mathrm{L}}\mathbf{u}_h + \beta_{x_\mathrm{L}}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\mathbf{u}_h - \mathbf{1}\mathcal{G}_{x_\mathrm{L}}\right), \\ \mathbf{SAT}_{x_\mathrm{R}} &= \sigma_{x_\mathrm{R}}\mathsf{H}^{-1}\mathsf{E}_{x_\mathrm{R}}\left(\alpha_{x_\mathrm{R}}\mathbf{u}_h + \beta_{x_\mathrm{R}}\mathsf{B}\mathsf{D}_{1,\mathrm{b}}\mathbf{u}_h - \mathbf{1}\mathcal{G}_{x_\mathrm{R}}\right), \end{aligned} \tag{7.6}$$

where $\mathbf{1}$ is a vector of ones. The terms within the parentheses are an approximation of the boundary conditions; the rest of the SAT is constructed to allow the energy method to be applied, with the additional parameters σ chosen so that the method is stable (for more information about the SATs used in this section see [12]).

The extension to a multi-element approach necessitates SATs for inter-element coupling, in addition to the boundary SATs (7.6), and in this paper we use the Baumann-Oden type interface SATs [12]. Consider two abutting elements, with solution $\mathbf{u}_h$ in the left element and solution $\mathbf{v}_h$ in the right element. The SAT for the right boundary of the left element is [12]

$$\begin{aligned} \mathbf{SAT}_{\mathbf{u}_h} &= \sigma_1^{(\mathbf{u}_h)}\mathsf{H}_{\mathbf{u}_h}^{-1}\left(\mathsf{E}_{\mathbf{u}_h,x_\mathrm{R}}\mathbf{u}_h - \mathbf{t}_{\mathbf{u}_h,x_\mathrm{R}}\mathbf{t}_{\mathbf{v}_h,x_\mathrm{L}}^\mathrm{T}\mathbf{v}_h\right) \\ &+\sigma_2^{(\mathbf{u}_h)}\mathsf{H}_{\mathbf{u}_h}^{-1}\left(\mathsf{E}_{\mathbf{u}_h,x_\mathrm{R}}\mathsf{B}_{\mathbf{u}_h}\mathsf{D}_{1,\mathrm{b}\,\mathbf{u}_h}\mathbf{u}_h - \mathbf{t}_{\mathbf{u}_h,x_\mathrm{R}}\mathbf{t}_{\mathbf{v}_h,x_\mathrm{L}}^\mathrm{T}\mathsf{B}_{\mathbf{v}_h}\mathsf{D}_{1,\mathrm{b}\,\mathbf{v}_h}\mathbf{v}_h\right) \\ &+\sigma_3^{(\mathbf{u}_h)}\mathsf{H}_{\mathbf{u}_h}^{-1}\left(\mathsf{D}_{1,\mathrm{b}\,\mathbf{u}_h}\right)^\mathrm{T}\mathsf{B}_{\mathbf{u}_h}\left(\mathsf{E}_{\mathbf{u}_h,x_\mathrm{R}}\mathbf{u}_h - \mathbf{t}_{\mathbf{u}_h,x_\mathrm{R}}\mathbf{t}_{\mathbf{v}_h,x_\mathrm{L}}^\mathrm{T}\mathbf{v}_h\right), \end{aligned} \tag{7.7}$$

where the subscripts $\mathbf{u}_h$ and $\mathbf{v}_h$ are used to identify operators for the left and right elements, and

$$\begin{aligned} \mathsf{Q}_{\mathbf{u}_h} + \mathsf{Q}_{\mathbf{u}_h}^\mathrm{T} &= \mathsf{E}_{\mathbf{u}_h,x_\mathrm{R}} - \mathsf{E}_{\mathbf{u}_h,x_\mathrm{L}} = \mathbf{t}_{\mathbf{u}_h,x_\mathrm{R}}\mathbf{t}_{\mathbf{u}_h,x_\mathrm{R}}^\mathrm{T} - \mathbf{t}_{\mathbf{u}_h,x_\mathrm{L}}\mathbf{t}_{\mathbf{u}_h,x_\mathrm{L}}^\mathrm{T}, \\ \mathsf{Q}_{\mathbf{v}_h} + \mathsf{Q}_{\mathbf{v}_h}^\mathrm{T} &= \mathsf{E}_{\mathbf{v}_h,x_\mathrm{R}} - \mathsf{E}_{\mathbf{v}_h,x_\mathrm{L}} = \mathbf{t}_{\mathbf{v}_h,x_\mathrm{R}}\mathbf{t}_{\mathbf{v}_h,x_\mathrm{R}}^\mathrm{T} - \mathbf{t}_{\mathbf{v}_h,x_\mathrm{L}}\mathbf{t}_{\mathbf{v}_h,x_\mathrm{L}}^\mathrm{T}. \end{aligned} \tag{7.8}$$

The SAT for the left boundary of the right element is given as

$$\begin{aligned} \mathbf{SAT}_{\mathbf{v}_h} &= \sigma_1^{(\mathbf{v}_h)}\mathsf{H}_{\mathbf{v}_h}^{-1}\left(\mathsf{E}_{\mathbf{v}_h,x_\mathrm{L}}\mathbf{v}_h - \mathbf{t}_{\mathbf{v}_h,x_\mathrm{L}}\mathbf{t}_{\mathbf{u}_h,x_\mathrm{R}}^\mathrm{T}\mathbf{u}_h\right) \\ &+\sigma_2^{(\mathbf{v}_h)}\mathsf{H}_{\mathbf{v}_h}^{-1}\left(\mathsf{E}_{\mathbf{v}_h,x_\mathrm{L}}\mathsf{B}_{\mathbf{v}_h}\mathsf{D}_{1,\mathrm{b}\,\mathbf{v}_h}\mathbf{v}_h - \mathbf{t}_{\mathbf{v}_h,x_\mathrm{L}}\mathbf{t}_{\mathbf{u}_h,x_\mathrm{R}}^\mathrm{T}\mathsf{B}_{\mathbf{u}_h}\mathsf{D}_{1,\mathrm{b}\,\mathbf{u}_h}\mathbf{u}_h\right) \\ &+\sigma_3^{(\mathbf{v}_h)}\mathsf{H}_{\mathbf{v}_h}^{-1}\left(\mathsf{D}_{1,\mathrm{b}\,\mathbf{v}_h}\right)^\mathrm{T}\mathsf{B}_{\mathbf{v}_h}\left(\mathsf{E}_{\mathbf{v}_h,x_\mathrm{L}}\mathbf{v}_h - \mathbf{t}_{\mathbf{v}_h,x_\mathrm{L}}\mathbf{t}_{\mathbf{u}_h,x_\mathrm{R}}^\mathrm{T}\mathbf{u}_h\right). \end{aligned} \tag{7.9}$$

For the numerical studies in this paper, the following values for the boundary condition and SAT parameters, based on the analysis in [12], are used:

$$
\begin{aligned}
&\alpha_{x_{\mathrm{L}}} = a \qquad \beta_{x_{\mathrm{L}}} = -\mu \qquad \alpha_{x_{\mathrm{R}}} = 0 \qquad \beta_{x_{\mathrm{L}}} = \mu \\
&\sigma_{x_{\mathrm{L}}} = \tfrac{\mu}{\beta_{x_{\mathrm{L}}}} \qquad \sigma_{x_{\mathrm{R}}} = \tfrac{-\mu}{\beta_{x_{\mathrm{R}}}} \\
&\sigma_1^{(\mathbf{u}_h)} = \tfrac{a}{2} \qquad \sigma_2^{(\mathbf{u}_h)} = \mu \qquad \sigma_3^{(\mathbf{u}_h)} = -\mu - \sigma_2^{(\mathbf{u}_h)} \\
&\sigma_1^{(\mathbf{v}_h)} = \sigma_1^{(\mathbf{u}_h)} - a \quad \sigma_2^{(\mathbf{v}_h)} = \sigma_2^{(\mathbf{u}_h)} + \mu \qquad \sigma_3^{(\mathbf{v}_h)} = -\sigma_2^{(\mathbf{u}_h)}.
\end{aligned} \tag{7.10}
$$

The solution error is defined by

$$
\|\mathbf{e}\|_{\mathsf{H}} = \sqrt{\mathbf{e}^{\mathrm{T}} \bar{\mathsf{H}} \mathbf{e}}, \tag{7.11}
$$

where $\mathbf{e} = (\mathbf{u}_h - \mathbf{u}_a)$, $\mathbf{u}_a$ is the restriction of the analytical solution onto the grid, and $\bar{\mathsf{H}}$ is a diagonal matrix with the norm matrix, H, from each element along the diagonal.

Figures 1 through 4 present the convergence of the $\|\mathbf{e}\|_{\mathsf{H}}$ versus $\frac{1}{\mathrm{DOF}}$ as well as the cpu time to compute the left-hand side (LHS) of (7.5), where DOF stands for the number of degrees of freedom in the spatial operator. For operators implemented using the traditional finite-difference approach, the number of degrees of freedom is simply the number of nodes, while for element-type operators, it is the product of the number of elements and the number of nodes in each element. Table 3 gives the convergence rates, computed by determining the slope of the line of best fit through the points $(x, y) = (\log(h), \log(\|\mathbf{e}\|_{\mathsf{H}}))$ associated with the filled-in markers in the figures. For operators implemented using the traditional finite-difference approach, h is taken as the average spacing between nodes, i.e., $\frac{x_{\mathrm{R}} - x_{\mathrm{L}}}{N-1}$, while for elements, h is computed as the size of the element. In this paper, grid refinement using the traditional finite-difference approach is carried out by doubling the number of nodes, while grid refinement using the element approach is carried out by equally subdividing elements, starting with one element at the coarsest grid level.

For operators with a repeating interior point operator, Figures 1 through 3, two main trends emerge. First, implementing the operators using the traditional finite-difference approach significantly reduces the global error. Second, compatible and order-matched operators are more accurate and more efficient than the application of the first-derivative operator twice. Examining Table 3, we see that for the traditional finite-difference approach, the operators have a convergence rate of roughly the order of the second-derivative operator plus two, which is consistent with the theory of Svärd and Nordström [28]. In contrast, the convergence rates using the element approach are worse for even-order compatible and order-matched operators, while the order of accuracy of application of the first-derivative operator twice is unaffected. Overall, we find that hybrid Gauss-trapezoidal and hybrid Gauss-trapezoidal-Lobatto operators are more accurate and therefore, in most cases, more efficient than either the application of classical SBP first-derivative operators twice or their compatible and order-matched counterparts.

For element-type operators, our interest is first to verify that operators constructed by leveraging Theorem 5.5, i.e., the compatible and order-matched operators constructed on the Chebyshev-Gauss nodal distribution, have reasonable performance. Second, we want to determine if we can find operators that provide some advantage

over the commonly used Legendre-Gauss-Lobatto operators. Figure 4 demonstrates that the five-node Chebyshev-Gauss compatible and order-matched operator is more efficient than either the application of the first-derivative-twice on that same nodal distribution, or the four-node Legendre-Gauss-Lobatto operator. Moreover, the application of the first derivative twice Chebyshev-Gauss operator is more efficient than the Legendre-Gauss-Lobatto operator. In that same Figure, we see that both seven-node Chebyshev-Gauss operators are as efficient as the five-node Legendre-Gauss-Lobatto operator. Moreover, we find that all of the compatible and order-matched operators with a repeating interior point operator, implemented as elements, are significantly more efficient than the Legendre-Gauss-Lobatto operators.

One possible reason for some of the suboptimal convergence rates experienced either by the element-type operators or operators with a repeating interior point operator applied as elements may be related to our use of the Baumann-Oden [2] interface SATs. Previous studies using such SATs have also shown suboptimal convergence rates for pseudo-spectral operators [5, 6], and it is possible that the same mechanisms are at play here.

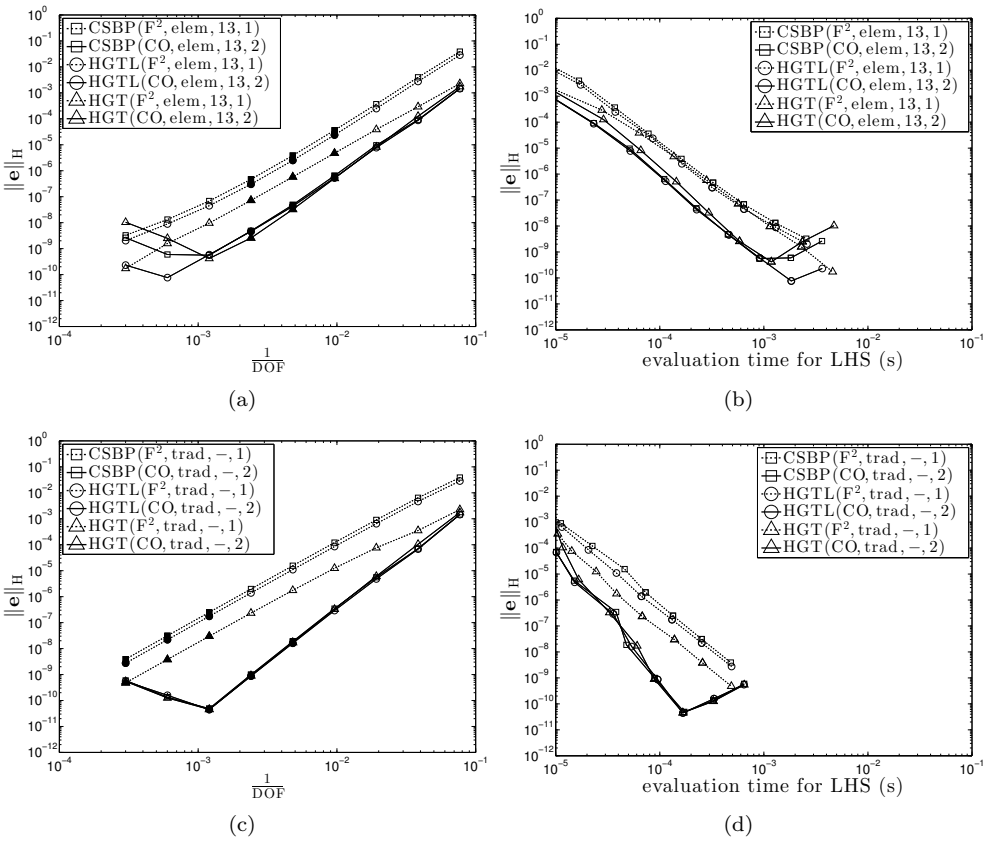

FIG. 1. *Solution error obtained using operators with a repeating interior point operator of order four implemented using the element approach or the traditional finite-difference approach.* H *norm of the error in the solution to problem (7.1) versus* $\frac{1}{\mathrm{DOF}}$*, (a) and (c), or versus cpu time to construct the LHS, (b) and (d). The hybrid Gauss-trapezoidal and hybrid Gauss-trapezoidal-Lobatto nodal distributions were constructed with* $a = j = 2$.

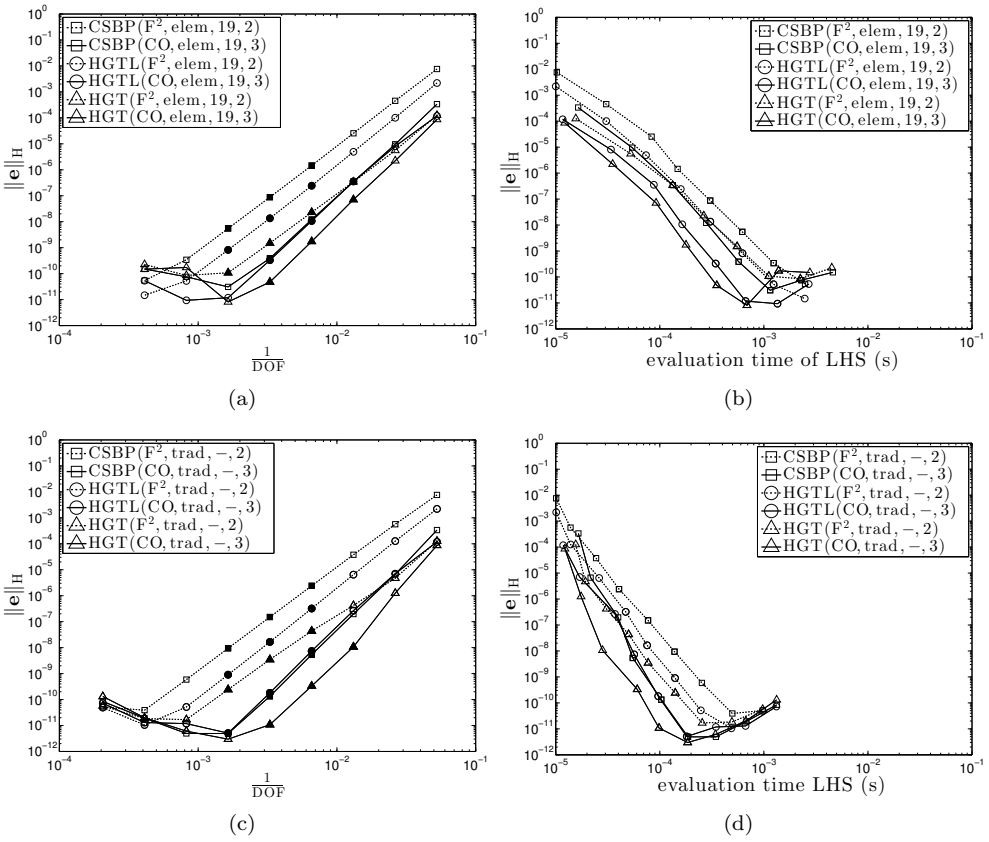

FIG. 2. *Solution error obtained using operators with a repeating interior point operator of order six using the element approach or the traditional finite-difference approach.* H *norm of the error in the solution to problem (7.1) versus* $\frac{1}{\mathrm{DOF}}$*, (a) and (c), or versus cpu time to construct the LHS, (b) and (d). The hybrid Gauss-trapezoidal and hybrid Gauss-trapezoidal-Lobatto nodal distributions were constructed with* $a = j = 3$.

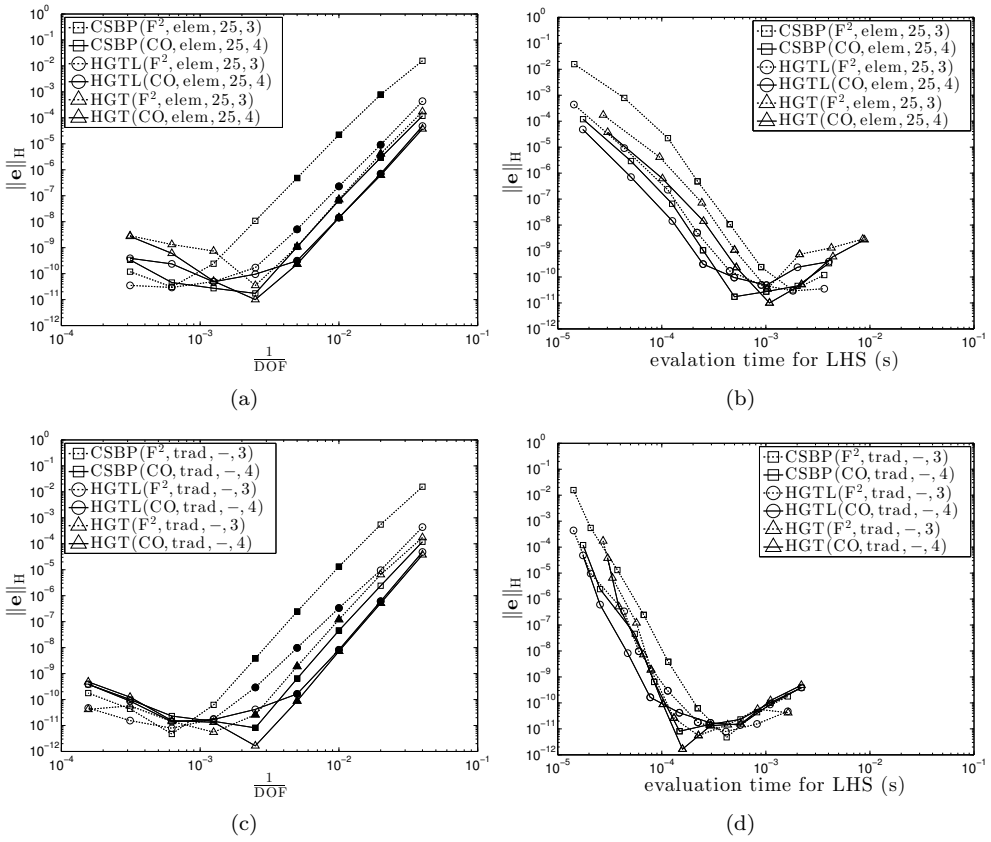

FIG. 3. *Solution error obtained using operators with a repeating interior point operator of order eight implemented using the element approach or the traditional finite-difference approach.* H *norm of the error in the solution to problem (7.1) versus* $\frac{1}{\mathrm{DOF}}$*, (a) and (c), or versus cpu time to construct the LHS, (b) and (d). The hybrid Gauss-trapezoidal and hybrid Gauss-trapezoidal-Lobatto nodal distributions were constructed with* $a = j = 4$*.*

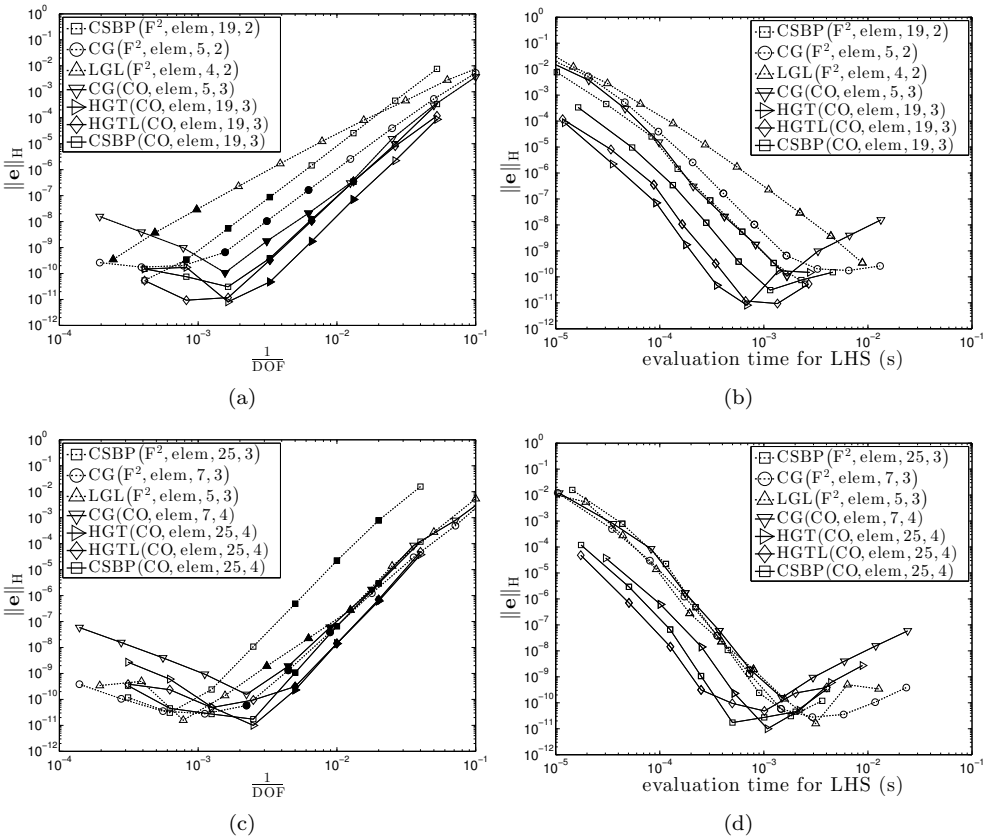

FIG. 4. *Comparison of various second-derivative operators of order two and three, (a) and (b), or three and four, (c) and (d).* H *norm of the error in the solution to problem (7.1) versus* $\frac{1}{\text{DOF}}$*, (a) and (c) or versus cpu time to construct the LHS, (b) and (d). The first-derivative operator in (a) and (b) is of order three and therefore the application of the first-derivative operator is of order two, while for (c) and (d) the first-derivative operator is of order four and therefore the application of the first-derivative twice is of order three.*

TABLE 3
Convergence of the H *norm of the error of the solution to problem (7.1) with a variable coefficient*

	Application of the first-derivative operator twice implemented using the element approach	Compatible and order-matched operators implemented using the element approach	Application of the first-derivative operator twice implemented using the traditional finite-difference approach	Compatible and order-matched operators implemented using the traditional finite-difference approach
Operator	$\mathrm{CSBP}\left(\mathrm{F}^2, \mathrm{elem}, 13, 1\right)$	$\mathrm{CSBP}(\mathrm{CO}, \mathrm{elem}, 13, 2)$	$\mathrm{CSBP}\left(\mathrm{F}^2, \mathrm{trad}, -, 1\right)$	$\mathrm{CSBP}(\mathrm{CO}, \mathrm{trad}, -, 2)$
Order	3.134	3.534	2.9939	4.2867
Operator	$\mathrm{HGTL}\left(\mathrm{F}^2, \mathrm{elem}, 13, 1\right)$	$\mathrm{HGTL}(\mathrm{CO}, \mathrm{elem}, 13, 2)$	$\mathrm{HGTL}\left(\mathrm{F}^2, \mathrm{trad}, -, 1\right)$	$\mathrm{HGTL}(\mathrm{CO}, \mathrm{trad}, -, 2)$
Order	3.1485	3.4247	2.9941	4.2364
Operator	$\mathrm{HGT}\left(\mathrm{F}^2, \mathrm{elem}, 13, 1\right)$	$\mathrm{HGT}(\mathrm{CO}, \mathrm{elem}, 13, 2)$	$\mathrm{HGT}\left(\mathrm{F}^2, \mathrm{trad}, -, 1\right)$	$\mathrm{HGT}(\mathrm{CO}, \mathrm{trad}, -, 2)$
Order	3.0184	3.8143	2.9815	4.2693
Operator	$\mathrm{CSBP}\left(\mathrm{F}^2, \mathrm{elem}, 19, 2\right)$	$\mathrm{CSBP}(\mathrm{CO}, \mathrm{elem}, 19, 3)$	$\mathrm{CSBP}\left(\mathrm{F}^2, \mathrm{trad}, -, 2\right)$	$\mathrm{CSBP}(\mathrm{CO}, \mathrm{trad}, -, 3)$
Order	4.027	4.8954	3.9855	5.0286
Operator	$\mathrm{HGTL}\left(\mathrm{F}^2, \mathrm{elem}, 19, 2\right)$	$\mathrm{HGTL}(\mathrm{CO}, \mathrm{elem}, 19, 3)$	$\mathrm{HGTL}\left(\mathrm{F}^2, \mathrm{trad}, -, 2\right)$	$\mathrm{HGTL}(\mathrm{CO}, \mathrm{trad}, -, 3)$
Order	4.1057	5.0385	4.2211	5.234
Operator	$\mathrm{HGT}\left(\mathrm{F}^2, \mathrm{elem}, 19, 2\right)$	$\mathrm{HGT}(\mathrm{CO}, \mathrm{elem}, 19, 3)$	$\mathrm{HGT}\left(\mathrm{F}^2, \mathrm{trad}, -, 2\right)$	$\mathrm{HGT}(\mathrm{CO}, \mathrm{trad}, -, 3)$
Order	3.8703	5.2723	3.7329	4.9415
Operator	$\mathrm{CSBP}\left(\mathrm{F}^2, \mathrm{elem}, 25, 3\right)$	$\mathrm{CSBP}(\mathrm{CO}, \mathrm{elem}, 25, 4)$	$\mathrm{CSBP}\left(\mathrm{F}^2, \mathrm{trad}, -, 3\right)$	$\mathrm{CSBP}(\mathrm{CO}, \mathrm{trad}, -, 4)$
Order	5.3374	5.7061	5.8418	6.1933
Operator	$\mathrm{HGTL}\left(\mathrm{F}^2, \mathrm{elem}, 25, 3\right)$	$\mathrm{HGTL}(\mathrm{CO}, \mathrm{elem}, 25, 4)$	$\mathrm{HGTL}\left(\mathrm{F}^2, \mathrm{trad}, -, 3\right)$	$\mathrm{HGTL}(\mathrm{CO}, \mathrm{trad}, -, 4)$
Order	5.4085	5.5649	5.0517	5.8663
Operator	$\mathrm{HGT}\left(\mathrm{F}^2, \mathrm{elem}, 25, 3\right)$	$\mathrm{HGT}(\mathrm{CO}, \mathrm{elem}, 25, 4)$	$\mathrm{HGT}\left(\mathrm{F}^2, \mathrm{trad}, -, 3\right)$	$\mathrm{HGT}(\mathrm{CO}, \mathrm{trad}, -, 4)$
Order	5.9434	5.6913	6.0576	6.1888
Operator	$\mathrm{CG}\left(\mathrm{F}^2, \mathrm{elem}, 5, 2\right)$	$\mathrm{CG}(\mathrm{CO}, \mathrm{elem}, 5, 3)$		
Order	3.9836	3.8073		
Operator	$\mathrm{LGL}\left(\mathrm{F}^2, \mathrm{elem}, 4, 2\right)$			
Order	3.1959			
Operator	$\mathrm{CG}\left(\mathrm{F}^2, \mathrm{elem}, 7, 3\right)$	$\mathrm{CG}(\mathrm{CO}, \mathrm{elem}, 7, 4)$		
Order	4.683	4.9015		
Operator	$\mathrm{LGL}\left(\mathrm{F}^2, \mathrm{elem}, 5, 3\right)$			
Order	3.5814			

8. Conclusions and future work. In this paper, we extended the generalized summation-by-parts operators developed in [7] to the second derivative with a constant or variable coefficient. We proposed definitions for operators that are one order more accurate than the application of the first-derivative operator twice, and in addition, operators that are compatible with the first-derivative operator. The principal conclusion that can be drawn from this paper is that it is possible to construct compatible and order-matched operators that are more accurate and efficient than the application of diagonal-norm classical SBP first-derivative operators twice. A future extension of this work is to multidimensional operators that can be applied to, for example, triangles and tetrahedra. Such operators are naturally used in the context of unstructured meshes and therefore represent a potentially effective strategy for the discretization of PDEs with second-derivative terms, such as the Navier-Stokes equations. Specific conclusions that can be drawn are:

- The hybrid Gauss-trapezoidal and hybrid Gauss-trapezoidal-Lobatto operators offer accuracy and efficiency gains relative to classical SBP operators.
- The compatible and order-matched versions of the above-mentioned GSBP operators, implemented as elements, are significantly more efficient than the examined Legendre-Gauss-Lobatto operators.
- Theorem 5.5 greatly simplifies the construction of compatible and order-matched GSBP operators, and the resultant operators are either more efficient or as efficient as the Legendre-Gauss-Lobatto operators.

Additional directions for future research include 1) to further explore element-type operators, for example using Alpert's quadrature rules to construct families of element-type operators; 2) to determine if more accurate and efficient element-type operators can be constructed by using the more general form of $\mathsf{R}(\mathsf{B})$; and 3) to determine whether using a different inter-element coupling SAT (for example see Refs. 5, 6, and 12) can improve the performance of compatible and order-matched operators.

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