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New Diagonal-Norm Summation-by-Parts Operators for the First Derivative with Increased Order of Accuracy

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In combination with simultaneous approximation terms, summation-by-parts (SBP) operators provide a flexible and efficient methodology that leads to consistent, conservative, and provably stable high-order discretizations. Traditional diagonal-norm SBP operators with a repeating interior point operator lead to solutions that have a global order of accuracy lower than the order of the interior point operator. A new family of diagonal-norm SBP operators is proposed that retains the order of accuracy of the interior operator. This new family of operators is compared to the traditional approach in the context of the linear convection equation, demonstrating a significant improvement in efficiency.

I. Introduction

The focus of this paper is on the development of summation-by-parts (SBP) operators¹⁻⁴ for the first derivative with a repeating interior point operator. Using simultaneous approximation terms (SATs)⁵⁻¹⁰ for the weak imposition of boundary conditions and inter-element coupling, the SBP-SAT approach leads to consistent, conservative, and provably stable discretizations of PDEs. Diagonal-norm SBP operators lead to stable discretizations in curvilinear coordinates.¹¹ Traditional diagonal-norm finite-difference SBP operators are of order 2p in the interior, while a number of boundary point operators are of order p, leading to errors in solutions of hyperbolic problems of global order p + 1.¹² The errors of traditional finite-difference-SBP operators can be reduced by considering operators that have nonuniform nodal distributions for a finite set of nodes at and near the boundaries.^{13, 14} However, the order of accuracy of these operators is not increased. The objective of this paper is to develop SBP operators where the order of the matrix operator matches the order of the interior point operator, potentially leading to more efficient discretizations.

The paper is organized as follows: in Section II, the notation used in the paper is given. SBP operators for the first derivative are reviewed in Section III. The development of the new family of SBP operators is detailed in Section IV, while Section V outlines specific steps to construct particular instances of these operators. In Section VI, a subset of the new family of SBP operators is compared to known SBP operators, in the context of the steady linear convection equation. Finally, conclusions are drawn in Section VII.

II. Notation and definitions

The conventions in this paper are a shortened version of those given are based on those laid out in Refs. 15, 3, and 16.

Vectors are denoted with small bold letters, for example, $\mathbf{x} = [x_1, \dots, x_N]^T$, 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 $x \in [x_L, x_R]$. As an example, $\mathcal{U}(x) \in C^{\infty}[x_L, x_R]$ denotes an infinitely differentiable function on the domain $x \in [x_L, x_R]$. Lower case bold font is 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

$$\mathbf{u} = \left[\mathcal{U}(x_1), \dots, \mathcal{U}(x_N)\right]^{\mathrm{T}}.$$
(1)

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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 $\mathbf{x}^k = \begin{bmatrix} x_1^k, \ldots, x_N^k \end{bmatrix}^{\mathrm{T}}$, with the convention that $\mathbf{x}^k = 0$ if k < 0. 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 operators. The approximation of the derivative has a leading truncation error term for each node, proportional to some power of h. The order of the operator is taken as the smallest exponent of h in these truncation errors. For operators approximating the first derivative, degree and order are equal.

III. Summation-by-parts operators for the first derivative

To motivate the definition of SBP operators for the first derivative, consider the unsteady linear-convection equation

$$\frac{\partial \mathcal{U}}{\partial t} = -\frac{\partial \mathcal{U}}{\partial x},\tag{2}$$

where $x \in [x_L, x_R]$, $t \ge 0$, and the initial and boundary conditions are not important for the current discussion. The energy method is applied to (2) in order to construct an energy estimate on the solution. This estimate is then used to determine stability (for more information regarding stability and the energy method, see Refs. 17, 18, and 19). The energy method consists of multiplying the PDE by the solution, integrating in space, transforming the integral on the RHS using integration-by-parts, and then integrating in time. This leads to

$$\|\mathcal{U}(\cdot,t)\|^{2} = \|\mathcal{U}(\cdot,0)\|^{2} - \int_{\tau=0}^{t} \mathcal{U}^{2}|_{x=x_{\mathrm{L}}}^{x_{\mathrm{R}}} \mathrm{d}\tau.$$
(3)

SBP operators for the first derivative are constructed such that when the energy method is applied to the semi-discrete or fully-discrete equations, energy estimates analogous to (3) can be constructed.

The equations that an order p SBP operator, D_x , approximating the first derivative must satisfy can be constructed using the restriction of monomials onto the grid. They are denoted the degree conditions and given as

$$\mathsf{D}_x \mathbf{x}^k = k \mathbf{x}^{k-1}, \quad k \in [0, p]. \tag{4}$$

For the first derivative, the above discussion leads to the following definition:^{3,4}

Definition 1 Summation-by-parts operator for the first derivative: A matrix operator $D_x \in \mathbb{R}^{N \times N}$ is an approximation to $\frac{\partial}{\partial x}$, on the uniform nodal distribution \mathbf{x} , of order p with the SBP property if

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

2. H, denoted the norm matrix, is symmetric positive definite; and

3.
$$\mathbf{Q} + \mathbf{Q}^{\mathrm{T}} = \mathbf{E} = \operatorname{diag}(-1, 0 \dots, 0, 1).$$

The operators originally developed by Kreiss and Scherer¹ and Strand² are referred to as classical finitedifference-SBP operators, which are characterized by a uniform nodal distribution that includes both boundary nodes and a repeating interior point operator. It is possible to extend the SBP idea to a broader set of operators by considering the construction of SBP operators on more general nodal distributions. For example, Carpenter and Gottlieb²⁰ proved that using the Lagrangian interpolant, operators with the SBP property can be constructed on nearly arbitrary nodal distributions. In related work, Gassner²¹ used these same ideas to interpret the discontinuous Galerkin spectral element method on the Legendre-Gauss-Lobatto quadrature nodes as a diagonal-norm SBP SAT method. These ideas led to generalized SBP (GSBP) operators, where the nodal distribution can be nonuniform and can exclude one or both boundary nodes.¹⁶ The required change in Definition 1 for a GSBP operator is to define E such that

$$\mathbf{x}_{j}^{\mathrm{T}}\mathsf{E}\mathbf{x}_{i} = x_{\mathrm{R}}^{i+j} - x_{\mathrm{L}}^{i+j}, \quad i, j \in [0, r], \quad r \ge p.$$
 (5)



Figure 1. Classical form of Q.

We describe an SBP or GSBP operator with a repeating interior point operator as a block operator. They are normally implemented using the traditional finite-difference approach where mesh refinement is accomplished by increasing the number of mesh nodes where the repeating interior point operator is applied. Conversely, a GSBP operator with no repeating interior point operator, denoted element-type operators, must be implemented using the element approach where *h*-refinement is carried out by increasing the number of elements while maintaining the element size. Note that a block operator can also be implemented as an element-type operator. However, the new family of SBP and GSBP operators with a repeating interior point operator considered here must necessarily be applied as elements; the reasons are discussed below.

IV. Form of new operators with order of accuracy of 2p

The goal of this paper is to construct SBP operators with a repeating interior point operator that are of order 2p everywhere by proposing a modification to the form of diagonal-norm SBP operators. We first discuss the construction of diagonal-norm classical finite-difference SBP operators and then their modification such that the resultant operator has the same order of accuracy at boundary nodes as in the interior. Consider such an operator for p = 2 on 12 nodes; thus, the repeating interior point operator is of order 2p = 4 and the boundary point operators are of order p = 2. The norm matrix is given as

$$\mathbf{H} = h \operatorname{diag} \left(h_{11}, h_{22}, h_{33}, h_{44}, 1, \dots, 1, h_{44}, h_{33}, h_{22}, h_{11} \right), \tag{6}$$

where h is the mesh spacing. The matrix Q has the form given in Figure 1, where M is nearly skew symmetric as shown. The repeating interior point operator is highlighted in blue, while the green triangles have entries that originate from the repeating interior point operator and ensure that the resultant Q is nearly skew symmetric. To apply this operator on a nodal distribution with more than 12 nodes, the matrix is expanded by inserting additional interior point operators, which does not require a change to the boundary point operators. In this example, there are 2p = 4 boundary point operators at either boundary, and this is the minimum required.² The number of boundary point operators can be increased by increasing the size of M; this has the potential to result in boundary point operators with significantly reduced truncation error.¹³ The entries in M and H are specified by satisfying the degree conditions (4) and the constraint that H be positive definite.

The new operators of order 2p at all nodes are given by $\tilde{\mathsf{D}}_x = \tilde{\mathsf{H}}^{-1}\tilde{\mathsf{Q}}$, where

$$\tilde{\mathsf{H}} = h \operatorname{diag} \left(\tilde{h}_{11}, \tilde{h}_{22}, \tilde{h}_{33}, \tilde{h}_{44}, 1, \dots, 1, \tilde{h}_{44}, \tilde{h}_{33}, \tilde{h}_{22}, \tilde{h}_{11} \right), \tag{7}$$

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	$-\frac{1}{2}$	\tilde{q}_{12}	\tilde{q}_{13}	\tilde{q}_{14}	0	0	0	0	c_{11}	c_{12}	c_{13}	c_{14}
	$-\tilde{q}_{12}$	0	\tilde{q}_{23}	\tilde{q}_{24}	0	0	0	0	c_{21}	c_{22}	c_{23}	c_{13}
$\tilde{Q} =$	$-\tilde{q}_{13}$	$-\tilde{q}_{23}$	0	\tilde{q}_{34}	$-\frac{1}{12}$	0	0	0	c_{31}	c_{32}	c_{22}	c_{12}
	$-\tilde{q}_{14}$	$-\tilde{q}_{24}$	$-\tilde{q}_{34}$	0	$\frac{2}{3}$	$-\frac{1}{12}$	0	0	c_{41}	c_{31}	c_{21}	c_{11}
	0	0	$\frac{1}{12}$	$-\frac{2}{3}$	0	$\frac{2}{3}$	$-\frac{1}{12}$	$\searrow 0$	0	0	0	0
	0	0	0	$\frac{1}{12}$	$-\frac{2}{3}$	0	$\frac{2}{3}$	$-\frac{1}{12}$	$\searrow 0$	0	0	0
	0	0	0	0	$\frac{1}{12}$	$-\frac{2}{3}$	0	$\frac{2}{3}$	$-\frac{1}{12}$	$\searrow 0$	0	0
	0	0	0	0	0	$\frac{1}{12}$	$-\frac{2}{3}$	0	$\frac{2}{3}$	$-\frac{1}{12}$	$\searrow 0$	0
	$-c_{11}$	$-c_{21}$	$-c_{31}$	$-c_{41}$	0	0	$\frac{1}{12}$	$-\frac{2}{3}$	0	\tilde{q}_{34}	\tilde{q}_{24}	\tilde{q}_{14}
	$-c_{12}$	$-c_{22}$	$-c_{32}$	$-c_{31}$	0	0	0	$\frac{1}{12}$	$-\tilde{q}_{34}$	0	\tilde{q}_{23}	\tilde{q}_{13}
	$-c_{13}$	$-c_{23}$	$-c_{22}$	$-c_{21}$	0	0	0	d	$-\tilde{q}_{24}$	$-\tilde{q}_{23}$	0	\tilde{q}_{12}
	$-c_{14}$	$-c_{13}$	$-c_{12}$	$-c_{11}$	0	0	0	0	$-\tilde{q}_{14}$	$-\tilde{q}_{13}$	$-\tilde{q}_{12}$	$\frac{1}{2}$
I	-	(-0	\tilde{C}^T									

Figure 2. Modified form of Q.

and \tilde{Q} has the form given in Figure 2, where the matrix \tilde{C} is constructed such that that the resultant operator satisfies the asymmetry of the first derivative under a reflection of the x-axis, that is, $\tilde{x} = -x$ leads to $\frac{\partial}{\partial x} = -\frac{\partial}{\partial \tilde{x}}$. The entries in \tilde{M} are not, in general, equal to those in M from the unmodified Q and similarly the entries in \tilde{H} are not the same as in H. The addition of the \tilde{C} matrix allows the construction of operators that are of order 2p everywhere. The entries in \tilde{C} are dependent on the number of nodes in the block. Therefore such an operator must be implemented as an element-type operator. This means that distinct operators must be constructed for each block size.

V. Construction of new operators with order of accuracy 2p

One of the difficulties in deriving SBP operators is satisfying the positive-definite constraint on H. We have found that restricting the number of non-unity weights in $\frac{1}{h}$ H to 2p at either boundary and first solving for H results in a positive-definite H for the operators presented in this paper. The diagonal norm matrix of an SBP operator of degree 2p has nonzero coefficients that result in a degree 4p - 1 quadrature rule;¹⁶ therefore, H must satisfy

$$\mathbf{1}^{\mathrm{T}}\mathsf{H}\mathbf{x}^{k} - \frac{\left(x_{\mathrm{R}}^{k+1} - x_{\mathrm{L}}^{k+1}\right)}{k+1} = 0, \ k \in [0, 4p-1].$$
(8)

The solution to (4) typically results in free parameters that enable optimization. The norm matrix of an order 2p SBP operator is a degree 4p - 1 approximation to the L_2 inner product^{16,22} and is used to compute functionals of the solution. Therefore, here the discrete SBP inner product of the error is used as the objective function, which for the first-derivative operator, \tilde{D}_x , is given as

$$J_{\mathbf{e}} = \mathbf{e}_{2p+1}^{\mathrm{T}} \tilde{\mathbf{H}} \mathbf{e}_{2p+1},\tag{9}$$

where the error vector is given as

$$\mathbf{e}_{2p+1} = \tilde{\mathsf{D}}_x \mathbf{x}^{2p+1} - (2p+1) \, \mathbf{x}^{2p}.$$
(10)

Without additional constraints, some of the operators that result have very large coefficients. These operators can be highly susceptible to round-off error. Therefore, in addition to (9), we use a second objective function, $J_{\tilde{Q}}$, which is the sum of the squares of the entries of \tilde{Q} . Maple's[©] minimize function is used to determine the minimum of objective function (9). Free parameters that do not affect J_{e} are used to minimize $J_{\tilde{Q}}$.

The steps to construct an order 2p operator are thus:

- Specify the number of nodes.
- Solve for the quadrature rule using (8) with \tilde{H} constructed to have 2p non-unity weights at the first and last 2p nodes. It is necessary to check that the resulting \tilde{H} is positive definite (for the operators considered in this paper we did not encounter negative or zero weights).
- Construct \hat{Q} and solve the degree conditions (4).
- Optimize the free parameters using objective J_e and specify the remaining free parameters by optimizing using objective J₀.

The above steps are sufficient for the operators considered in this paper. However, for even higher order operators, it may be the case that $\frac{1}{h}\tilde{H}$ will require greater than 2p non-unity weights at the first and last number of nodes in order to satisfy the positive definite constraint; similarly, \tilde{M} and \tilde{C} might need to be expanded.

Up to this point we have used the $\tilde{}$ to differentiate between the constituent matrices of operators with and without the corner correction, to make clear that the entries in these matrices are different. Since this is now clear, we no longer make this distinction.

In addition to SBP operators constructed on uniform nodal distributions, we investigate GSBP operators with a repeating interior point operator that have a number of nodes at the boundaries that are not uniformly spaced. By allowing the nodal distribution to vary near the boundary, it is possible to construct operators with reduced error but with no effect on the order of accuracy.¹³

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.¹³ Instead, for diagonal-norm SBP operators, it is possible to start with a quadrature rule with positive weights and then construct the norm matrix by injecting the weights of the quadrature rule along the diagonal.¹⁶ Quadrature rules on nodal distributions that have a number of unequally spaced nodes at and near boundaries with equally spaced interior nodes were proposed by Alpert²³ and have been successfully used to construct GSBP operators.¹⁴ The nodal locations and quadrature weights are derived from the solution to

$$\sum_{i=1}^{j} \tilde{w}_{i} \tilde{x}_{i}^{r} = \frac{B_{r+1}(a)}{r+1}, \quad r = 0, 1, \dots, 2j - 2,$$
(11)

 $\tilde{x}_0 = 0,$

where $B_i(x)$ is the *i*th Bernoulli polynomial, $B_0(x) = 1$, and the last equation ensures that nodes at the boundaries are included. The resultant nodal distribution is referred to as the hybrid Gauss-trapezoidal-Lobatto (HGTL) nodal distribution. The parameters a and j are chosen so that a particular degree is attained. For the nodal distributions considered by Alpert,²³ choosing a = j results in quadrature rules with positive weights up to degree 20.²³ We therefore choose a = j. To construct a nodal distribution on $x \in [0, 1]$, the following relations are used:

$$x_{i} = h\tilde{x}_{i}, \quad x_{N-(i-1)} = 1 - h\tilde{x}_{i}, \quad i \in [1, j],$$

$$x_{i+j+1} = h(a+i), \quad i \in [0, n-1],$$
(12)

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

Rather than using the quadrature rules given by Alpert,²³ we use the nodal distributions that result from (11) and construct operators with Q or \tilde{Q} on these nodal distributions using the previously described steps. Table 1 summarizes the various operators considered in this paper. The HGTL2, HGTLC25_4, HGTLC50_4, HGTLC25_6, and HGTLC50_6 operators are constructed on the HGTL nodal distribution derived from (11) for a = j = 2, while the HGTL3 operator is constructed on the HGTL nodal distribution for a = j = 3.

Table 1. Abbreviations for GSBP operators for the second derivative

Abbreviation	Operator
$\mathrm{CSBP}[p]$	Order p classical finite-difference-SBP operator with a repeating interior point
	operator of order $2p$
$\text{CSBPC}[N]_{-}[2p]$	Order p classical finite-difference-SBP operator on N nodes with a repeating
	interior point operator of order $2p$ constructed using \tilde{Q}
$\mathrm{HGTL}[p]$	Order p GSBP operator with a repeating interior point operator of order $2p$
	constructed on the HGTL nodes using Q
$\mathrm{HGTLC}[N]_{-}[2p]$	Order $2p$ GSBP operator on N nodes with a repeating interior point operator
	of order $2p$ constructed on the HGTL nodes using \tilde{Q}

VI. Results

In this section, a steady form of the linear convection equation with a source term is used as a testbed to characterize the proposed operators. The continuous problem is given as

$$-\frac{\partial \mathcal{U}}{\partial x} + \mathcal{S} = 0, \ x \in [0, 1], \tag{13}$$

where \mathcal{S} is a source term such that

$$\mathcal{U}(x,t) = 1 + \left(\left(-32\,x + 16 \right) \sin\left(10\,\pi\,x \right) + 10\,\cos\left(10\,\pi\,x \right) \pi \right) e^{-4\left(2\,x - 1 \right)^2} \tag{14}$$

is a solution to (13). The boundary condition is given as

$$\mathcal{U}(0) = \mathcal{G}_0,\tag{15}$$

where $\mathcal{G}_0(t)$ is constructed such that (14) is the solution to (13). The discrete H norm of the error of the solution is computed using

$$\|\mathbf{e}\|_{\mathsf{H}} = \mathbf{e}^{\mathrm{T}}\mathsf{H}\mathbf{e},\tag{16}$$

where $\mathbf{e} = \mathbf{u}_h - \mathbf{u}$, \mathbf{u}_h is the discrete solution, and \mathbf{u} is the projection of exact solution onto the nodal distribution. The discrete equations are given as

$$-\mathsf{D}_x \mathbf{u}_h + \mathbf{s} + \mathbf{SAT}_{\mathrm{BC}} + \mathbf{SAT}_{\mathrm{I}} = 0, \tag{17}$$

where s is the projection of the source term onto the nodal distribution. The term \mathbf{SAT}_{BC} is to enforce the boundary condition, while the term \mathbf{SAT}_{I} is used to enforce the inter-element coupling (for more information about SATs see Refs. 5, 6, 7, 8, 24, 25, 26, 27, and 28). The CSBP and HGTL operators are applied using an element approach with blocks of 50 nodes.

Figures 3(a) and 4(a) depict the convergence of $\|\mathbf{e}\|_{\mathsf{H}}$, while Tables 2 and 3 give 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 with p = 2 (Table 2), the new operators demonstrate convergence rates approximately two orders higher then both the classical SBP operator and the HGTL operator. The p = 3 operators (Table 3), display convergence rates that are approximately 3 orders higher. Figures 3(a) and 4(a) show that the new operators lead to reduced errors as well. Figures 3(b) and 4(b) show the convergence of $\|\mathbf{e}\|_{\mathsf{H}}$ as a function of floating point operations (FLOs) and it can be seen that the new operators are more efficient than either the CSBP or HGTL operators for error tolerances below a certain threshold.

The new operators require a small increase in the number of FLOs for a given element size. Figures 2(c) and 3(c) show the relative efficiency of the various operators compared to the CSBP operators. The new operators, for p = 2 (Figure 2(c)), are increasingly more efficient for error tolerances smaller than 10^{-4} . Similarly, for the p = 3 operators (Figure 3(c)), the new operators are increasingly more efficient for error tolerances smaller than 10^{-5} . In contrast to the p = 2 operator, the HGTL operator for p = 3 is significantly more efficient than the CSBP operator. For p = 3 the new operators are more efficient than HGTL for $||\mathbf{e}||_{\rm H}$ below 10^{-7} .

Operator	$\mathrm{Order} \; \ \mathbf{e}\ _{H}$
CBP2	3
HGTL2	3.0001
$CSBPC25_4$	4.9896
$CSBPC50_4$	5.0444
$\mathrm{HGTLC25}_{-4}$	4.802
HGTLC50_4	4.856

Table 2. Convergence rates of $\|\mathbf{e}\|_{\mathsf{H}}$ for operators with p = 2

Table 3. Convergence rates of $\|\mathbf{e}\|_{\mathsf{H}}$ for operators with p = 3

$\mathrm{Order} \; \ \mathbf{e}\ _{H}$
4.0031
4.0107
6.9847
7.3071
6.9856
7.3443

VII. Conclusions

We modify the structure of classical SBP operators such that a new family of operators can be constructed that has the same order at all nodes as the repeating interior point operator. The resultant operators are of order 2p and for the steady convection equation produce solutions of order 2p + 1, while the classical SBP operators are of order p and typically have solutions of order p + 1. For sufficiently tight error tolerances, the new family of corner-corrected operators has lower global error, better convergence rates, and is more efficient than either classical SBP operators or HGTL operators without the corner correction.



Figure 3. Operators with p = 2: a) Convergence of $\|\mathbf{e}\|_{\mathsf{H}}$ versus $\frac{1}{\mathsf{DOF}}$, b) Convergence of $\|\mathbf{e}\|_{\mathsf{H}}$ versus $\frac{1}{\mathsf{FLOs}}$, and c) floating point operations relative to the CSBP2 operator. Filled in markers are used in computing the convergence rates.



Figure 4. Operators with p = 3: a) Convergence of $||e||_{H}$ versus $\frac{1}{DOF}$, b) Convergence of the $||e||_{H}$ versus $\frac{1}{FLOS}$, and c) floating point operations relative to the CSBP3 operator. Filled in markers are used in computing the convergence rates.

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