

Multidimensional Diagonal-Norm Summation-by-Parts Operators on Quadrilateral Elements

Kevin J. Mattalo^{*} and David W. Zingg[†]

University of Toronto Institute for Aerospace Studies, Toronto, Ontario, M3H 5T6

The summation-by-parts (SBP) property provides a rigorous means of proving linear and nonlinear stability. Recently, the SBP property has been extended from tensor-product nodal distributions on multiblock curvilinear meshes to unstructured meshes on arbitrary polytopes. The objective of this paper is to search for efficient cubature rules on quadrilateral elements and perform a comparative analysis of their properties relative to traditional tensor-product operators. To this end, an algorithm for the constrained numerical optimization of multidimensional SBP operators on quadrilateral elements is presented. Using this algorithm, operators are optimized relative to an objective function which accounts for accuracy of the SBP derivative operator. Additionally, properties which affect time stability for explicit time integration methods and conditioning of the node set are calculated and analyzed. Properties necessary to preserve the SBP property are enforced through linear and nonlinear constraints. Numerical experiments are presented comparing tensor-product element-type operators on Legendre-Gauss (LG) and Legendre-Gauss-Lobatto (LGL) nodal distributions and non-tensor-product nodal distributions in order to understand the relative accuracy and computational efficiency of the corresponding methods. It is found that the non-tensor-product nodal distributions are able to achieve cubature rules with lower cubature truncation error compared to tensorproduct cubature rules, with fewer nodes. Additionally, the SBP operators constructed on the non-tensor-product cubature nodes are found to have equal or better solution error and efficiency for test cases performed with the linear advection and Euler equations on curvilinear grids.

I. Introduction

H^{IGH-ORDER} methods on unstructured meshes are a promising approach for the efficient solution of industrially relevant partial differential equations on massively parallel computer architectures. This is due to their high arithmetic intensity, ability to mesh complex geometries, low communication overhead between computational processes, and ability to obtain accurate computations with fewer degrees of freedom than a low-order method [1–3]. As a means to prove stability, the summation-by-parts (SBP) framework was developed, initially in the finite difference community, by Kreiss and Scherer [4] and then extended by Strand [5]. This framework was extended with the addition of simultaneous approximation terms (SATs) for the energy-stable weak imposition of interface coupling and boundary conditions [6, 7]. This methodology has been applied to complex practical problems in aerodynamics [8] and Einstein's equations in gravitational physics [9]. Beyond the finite difference context, the SBP property has also been used extensively within the high-order community for spectral [10], discontinuous Galerkin [11], finite volume [12], and flux reconstruction methods [13].

The ability of SBP-SAT schemes to provide provably stable and conservative discretizations of linear initial-valueproblems results from the discrete representation of integration-by-parts and its corresponding bilinear forms within the construction of the matrix operators. Traditionally, SBP operators on structured curvilinear grids are implemented as finite difference operators with uniform nodal distributions which contain boundary nodes. Mesh refinement is performed through the repetition of an order 2p repeating interior point operator finite difference stencil. To enforce the SBP property, order p corrections to the boundary stencils are introduced, which reduces the overall accuracy of the operator to p for diagonal-norm (mass) matrices. However, a recent extension of the SBP definition by Del Rey Fernández *et al.* allows for the construction of generalized summation-by-parts operators (GSBP) for the first and second

^{*}M.A.Sc Student, Institute for Aerospace Studies, 4925 Dufferin Street, and AIAA Student Member kevin.mattalo@mail.utoronto.ca

[†]University of Toronto Distinguished Professor of Computational Aerodynamics and Sustainable Aviation, Director, Centre for Research in Sustainable Aviation, Director, Centre for Computational Science and Engineering, Institute for Aerospace Studies, 4925 Dufferin Street, and AIAA Associate Fellow dwz@oddjob.utias.utoronto.ca

derivatives [14, 15]. The operators satisfying the GSBP definition include a wide variety of operators with the following properties:

- operators without a repeating interior point operator,
- operators that do not contain one or both of the boundary nodes,
- operators that have nonuniform nodal distributions.

The GSBP operators can be implemented as either element-type operators or traditional finite difference operators. Coupled with the inherent relationship between quadrature rules and SBP operators [16], the construction of high-order SBP operators reduces to finding a quadrature rule of sufficient degree. The extension to multiple dimensions can be performed through a simple tensor-product of the one-dimensional operator; however, recent extensions to multidimensional SBP operators on simplices [17] have been developed in addition to the generalization of SATs on arbitrary polytopes [18]. The flexibility and generality of the SBP definition has opened the question of which operators are *optimal* in terms of specific objectives such as the L^2 error, computational efficiency, and dispersion and dissipation error properties, and the procedures required to develop such operators.

Optimization of traditional one-dimensional diagonal-norm SBP finite difference schemes focused solely on the optimization of the free matrix parameters that appear after satisfying the accuracy equations and the SBP definition [5, 9, 19]. For these optimization cases, nodal distributions were assumed to be uniform and therefore no additional degrees of freedom were introduced into the SBP operator through the node position parameters. An extension of the optimization of one-dimensional diagonal-norm SBP operators was performed by Mattsson *et al.* for operators of orders p = 1, 2, 3, and 4 [20]. By implementing enlarged boundary stencils into the SBP matrix operators and setting the positions of some of the nodes near the boundary as free parameters in their optimization, they optimized their SBP operators to minimize the norm of the first two leading derivative truncation error terms. Their results showed multiple orders of magnitude improvement in the L^2 solution error for the Euler vortex problem over traditionally optimized diagonal-norm SBP finite difference methods containing a uniform nodal distribution. Revisiting this concept, Mattsson *et al.* performed an improved optimization of these operators for diagonal-norm SBP operators of orders p = 1, 2, 3, 4, 5and 6 [21]. By utilizing more non-uniform nodes near the boundary, they were able to improve the L^2 solution error for the Euler vortex problem compared to their operators from [20] and introduced *minimal* SBP operators which use the non-uniform nodes to reduce the size of the boundary closure to less than 2p for operators possessing a diagonal-norm.

For diagonal-norm multidimensional SBP operators that are exact for polynomials of degree p, it was shown by Del Rey Fernández *et al.* that the norm and corresponding nodes define a strong cubature rule that is exact for polynomials of at least degree 2p - 1 [17]. The analytic and algorithmic search for such cubature rules is documented extensively by Cools [22]. Additional investigations of efficient symmetric cubature rules over quadrilateral and hexahedral domains have been performed [23, 24]; however, these rules generally suffer from negative weights or possess node positions that are outside of the domain. For this reason, the use of cubature rules in multiple dimensions and for the solution nodes in collocation type discontinuous Galerkin spectral element methods on quadrilateral elements has resorted to the tensor-product of LG and LGL nodes for their proven interpolation and accuracy properties [11, 25, 26].

The current objective is to investigate the constrained numerical optimization of multidimensional SBP operators on quadrilateral elements and to compare their accuracy and computational efficiency to traditional node sets such as a tensor-product of LG or LGL nodes. We restrict ourselves to the study of diagonal-norm SBP operators. The numerical optimization approach performed in this paper is to first perform a nonlinear least-squares optimization procedure of a cubature rule with the constraint that the cubature rule node set is symmetric, contains positive weights, and is of a sufficient cubature degree on a quadrilateral element that contains either only volume nodes on the interior, volume nodes on the facets or interior, or volume nodes collocated with the facet cubature rule belonging to each SBP operator family so that an SBP operator can be directly constructed, although we do not claim that these cubature rules are new. Given the cubature rule and subsequently solving the accuracy conditions, free matrix parameters can appear in the SBP operators which can be optimized for specific objective functions that account for accuracy, time stability for explicit time integration methods, and computational cost, or a weighted linear combination of such parameters. Similar procedures have been performed in [20, 21, 27].

A brief outline of the multidimensional SBP operator theory will be followed by a description of the current classes of multidimensional SBP operator families and their properties. A procedure for numerically optimizing cubature rules on quadrilateral elements will then be discussed, and an extensive list of the generated cubature rules for each SBP family will be presented. A detailed outline of how the SBP operators are constructed while retaining free parameters in the matrix operators follows. Subsequently, the objective functions and their influences on specific SBP operator properties will be provided in addition to the description of the optimization algorithms and procedure. Following this, a comparison of the various classes and families of optimized multidimensional SBP operators on quadrilaterals to traditional tensor-product operators will be presented. Finally, a comparison of the accuracy and computational efficiency of the tensor-product and multidimensional operators when applied to canonical test problems for the linear advection and Euler equations on curvilinear grids will be presented.

II. Notation

Adopting conventions established in [17, 18], the following notation is used throughout the paper. We consider discretized operators defined on a set of *n* nodes $S_{\hat{\Omega}} = \{(\xi_i, \eta_i)\}_{i=1}^n$, on an open and bounded domain $\hat{\Omega} \subset \mathbb{R}^2$. Capital letters with a script type are used to denote continuous functions defined on the domain $\hat{\Omega}$. As an example, $\mathcal{U}(\xi) \in L^2(\hat{\Omega})$ is a square-integrable function defined in the domain $\hat{\Omega}$. Additionally, lower-case bold font is used to denote the restriction of functions to the node set $S_{\hat{\Omega}}$. Therefore, the restriction of the function \mathcal{U} to $S_{\hat{\Omega}}$ is represented as

$$\mathbf{u} = [\mathcal{U}(\xi_1, \eta_1), \dots, \mathcal{U}(\xi_n, \eta_n)]^{\mathrm{T}}.$$

Various definitions and theorems will also rely on a monomial basis. The cardinality of the monomial basis for arbitrary dimension d and degree p is given as

$$n_p^* \equiv \binom{p+d}{d}.$$

The monomial basis functions are represented as

$$\mathcal{P}_k(\xi,\eta) = \xi^i \eta^j, \qquad k = j(j+1)/2 + i + 1 \quad \forall j \in \{0,1,\dots,p\}, \quad i \in \{0,1,\dots,j\},$$

and the evaluation of the monomials and their derivatives on the node set $S_{\hat{\Omega}}$ is given as

$$\mathbf{p}_{k} \equiv [\mathcal{P}_{k}(\xi_{1},\eta_{1}),\ldots,\mathcal{P}_{k}(\xi_{n},\eta_{n})]^{\mathrm{T}},$$

and
$$\mathbf{p}_{k}' \equiv \left[\frac{\partial \mathcal{P}_{k}}{\partial \xi}(\xi_{1},\eta_{1}),\ldots,\frac{\partial \mathcal{P}_{k}}{\partial \xi}(\xi_{n},\eta_{n})\right]^{\mathrm{T}}.$$

Matrices are represented using capital letters with sans serif font; for example, the first-derivative operators with respect to ξ and η are represented by the matrices D_{ξ} and D_{η} , respectively. Entries of a matrix are indicated with subscripts, and we follow a MATLAB-like notation when referencing submatrices. For example, $A_{:,j}$ represents the j^{th} column of matrix A.

We will also require the degree p (rectangular) Vandermonde matrix

$$\mathsf{V}\equiv\Big[\mathbf{p}_1,\mathbf{p}_2,\ldots,\mathbf{p}_{n_p^*}\Big],$$

as well as the associated matrix containing the projection of the ξ derivatives of the monomials onto S_{Ω} , denoted by

$$\mathsf{V}_{\xi} \equiv \left[\mathbf{p}_{1}^{\prime}, \mathbf{p}_{2}^{\prime}, \dots, \mathbf{p}_{n_{p}^{*}}^{\prime}\right].$$

III. Multidimensional Summation-by-Parts Operators

A. Multidimensional Summation-by-Parts Operator Approximating the First-Derivative

To introduce the definition of a multidimensional summation-by-parts operator approximating the first-derivative, consider a domain $\Omega \subset \mathbb{R}^2$ with a piecewise-smooth boundary Γ . Given a set of points $\{a_0, \ldots, a_n\}$ in \mathbb{R}^2 such that the vectors $\{a_1 - a_0, \ldots, a_d - a_0\}$ are linearly independent, then the interior of the convex hull of $\{a_0, \ldots, a_n\}$ is a non-degenerate polygon in \mathbb{R}^2 . We then consider a partition $\mathcal{T} = \{T\}$ of the domain Ω which is a collection of disjoint and non-degenerate polygons such that

$$\Omega = \bigcup_{T \in \mathcal{T}} T.$$

Each $T \in \mathcal{T}$ is defined as a mesh element [28].

Consider now the two-dimensional scalar conservation law given by

$$\frac{\partial \mathcal{U}}{\partial t} + \frac{\partial \mathcal{U}}{\partial x} + \frac{\partial \mathcal{U}}{\partial y} = 0, \quad \forall x, y \in \Omega, \quad t \ge 0.$$
(1)

Using the partition \mathcal{T} of Ω , each mesh element T can be mapped from physical coordinates (x, y) to a reference polygon in computational coordinates (ξ, η) through a mapping. This mapping results in the following modification to Eq. (1):

$$\frac{\partial(\mathcal{J}^{-1}\mathcal{U})}{\partial t} + \frac{\partial(\lambda_{\xi}\mathcal{U})}{\partial\xi} + \frac{\partial(\lambda_{\eta}\mathcal{U})}{\partial\eta} = 0,$$
(2)

where λ_{ξ} and λ_{η} are the metrics and \mathcal{J} is the Jacobian of the transformation. Now that Eq. (2) is written in the computational domain, the corresponding metric relations can be calculated and the terms $\frac{\partial}{\partial \xi}$ and $\frac{\partial}{\partial \eta}$ can be approximated by discrete first-derivative matrix operators D_{ξ} and D_{η} , respectively.

Definition 1. Multidimensional summation-by-parts operator for the first-derivative: Consider an open and bounded domain $\hat{\Omega} \subset \mathbb{R}^2$ with a piecewise-smooth boundary $\hat{\Gamma}$ which belongs to the associated partition \mathcal{T} of Ω . The matrix D_{ξ} is a degree *p* SBP approximation to the first-derivative $\frac{\partial}{\partial \xi}$ on the nodes $S_{\hat{\Omega}} = \{(\xi_i, \eta_i)\}_{i=1}^n$ if

- 1) $\mathsf{D}_{\xi}\mathbf{p}_{k} = \mathbf{p}_{k}', \quad \forall k \in \{1, 2, \dots, n_{p}^{*}\};$
- 2) $D_{\xi} = H_{-}^{-1}Q_{\xi}$, where H is symmetric positive-definite; and
- 3) $Q_{\xi} + Q_{\xi}^{T} = E_{\xi}$, where E_{ξ} is a discrete representation of a directional surface integral such that

$$\mathbf{p}_k^{\mathrm{T}} \mathsf{E}_{\xi} \mathbf{p}_m = \oint_{\hat{\Gamma}} \mathcal{P}_k \mathcal{P}_m n_{\xi} d\hat{\Gamma}, \quad \forall k, m \in \{1, 2, \dots, n_r^*\},$$

where $r \ge p$, and n_{ξ} is the ξ component of the outward pointing unit normal on $\hat{\Gamma}$, $\mathbf{n} = [n_{\xi}, n_n]^{\mathrm{T}}$.

It is clear from the above definition that the SBP operators are discretely mimetic of integration-by-parts and the corresponding bilinear forms present. We say that an SBP operator is a diagonal-norm SBP operator if H is a diagonal matrix. As stated in the Introduction, the existence of a cubature rule of sufficient degree is necessary and sufficient for the existence of a multidimensional diagonal-norm SBP operator [17]. In this case, the norm matrix H contains the cubature weights $\omega = {\omega_1, \ldots, \omega_n}$ injected on the diagonal entries. Consequently, H is a cubature rule satisfying

$$\mathbf{p}_k^{\mathrm{T}} \mathsf{H} \mathbf{p}_m = \int_{\hat{\Omega}} \mathcal{P}_k \mathcal{P}_m d\hat{\Omega},$$

where H contains the weights of a cubature rule of at least degree 2p - 1. As H is symmetric positive-definite, it is a degree 2p - 1 finite-dimensional representation of the L^2 norm

$$||\mathbf{u}||_{\mathsf{H}}^2 \equiv \mathbf{u}^{\mathrm{T}}\mathsf{H}\mathbf{u} \approx \int_{\hat{\Omega}} \mathcal{U}^2 d\hat{\Omega}.$$

Furthermore, the construction of the directional surface integral was generalized in [18] through the decomposition of the E_{ξ} operator. First, we begin by assuming that the reference element $\hat{\Omega}$ is a polygon, and its boundary $\hat{\Gamma}$ is piecewise-smooth with $\hat{\Gamma} = \bigcup_{j=1}^{n_{\Gamma}} \hat{\Gamma}_j$ and $\bigcap_{j=1}^{n_{\Gamma}} \hat{\Gamma}_j = \emptyset$. For each $\hat{\Gamma}_j$ we also assume there exists a strong cubature rule, with nodes $S_{\hat{\Gamma}_j} = \{(\xi_i, \eta_i)\}_{i=1}^{n_j}, n_j \ge p + 1$, and weights $\{b_i^{(j)}\}_{i=1}^{n_j}$ that exactly integrates polynomial integrands of degree $q \ge 2r$ on each facet, where *r* is used in property III of Definition 1. In addition, we assume that the volume nodes generate a degree *r* Vandermonde matrix V, which has full rank.

Using the above assumptions, a simple decomposition of E_{ξ} involves projecting the solution at the volume nodes onto the facet cubature nodes, integrating over the facet and multiplying pointwise by the local normal component in the ξ direction, and then projecting from the facet cubature nodes back onto the volume nodes. The projection from the volume nodes to the facet cubature nodes is performed by the operator R_j , which is accurate to degree $r \ge p$ and obeys the property

$$(\mathsf{R}_{j}\mathbf{p}_{k})_{i} = \mathcal{P}_{k}(\xi_{i}^{(j)},\eta_{i}^{(j)}), \quad i = 1, 2, \dots, n_{j}, \quad \forall k \in \{1, 2, \dots, n_{r}^{*}\},$$

Families	Can contain volume nodes on interior	Can contain volume nodes on boundary	Volume nodes collocated with facet cubature	Diagonal E
SBP-Ω [18]	✓	×	×	X
SBP-Γ [17]	1	1	×	×
SBP-diag(E) [29]	1	1	✓	1

where $r \ge p$. We can now write the decomposition of $\mathsf{E}_{\mathcal{E}}$ as

$$\begin{split} \mathsf{E}_{\xi} &= \sum_{j=1}^{n_{\hat{\Gamma}_j}} \mathsf{R}_j^{\mathsf{T}} \mathsf{B}_j \mathsf{N}_{\xi j} \mathsf{R}_j, \\ \mathsf{R}_j &= \mathsf{V}_{\hat{\Gamma}_j} (\mathsf{V}_{\hat{\Omega}})^{\dagger} = \mathsf{V}_{\hat{\Gamma}_j} (\mathsf{V}_{\hat{\Omega}}^{\mathsf{T}} \mathsf{V}_{\hat{\Omega}})^{-1} \mathsf{V}_{\hat{\Omega}}^{\mathsf{T}} \end{split}$$

where $B_j = \text{diag}(b_1^{(j)}, b_2^{(j)}, \dots, b_{n_j}^{(j)})$ is a diagonal matrix holding the quadrature weights for $\hat{\Gamma}_j$ and $N_{\xi j} = \text{diag}(n_{\xi 1}^{(j)}, n_{\xi 2}^{(j)}, \dots, n_{\xi n_j}^{(j)})$ is a diagonal matrix holding the ξ component of the normal vector at each quadrature point on $\hat{\Gamma}_j$. The matrix $V_{\hat{\Omega}}$ is a degree *r* Vandermonde matrix on the volume nodes and the matrix $V_{\hat{\Gamma}_j}$ is a degree *r* Vandermonde matrix on the facet *j* quadrature nodes. A similar decomposition can be made in the η direction.

B. Multidimensional Summation-by-Parts Operator Families

Currently, there exist three primary families of multidimensional SBP operators in which we can classify many multidimensional SBP operators. These families are the SBP- Ω , SBP- Γ , and SBP-diag(E) families. These families determine the structure of the volume node set within the reference element $\hat{\Omega}$ and hence the matrix structure of the corresponding SBP operator. Although these families have only been constructed for simplices, the extension to quadrilateral and hexahedral elements is straightforward. A summary of the differences between the different families is given in Table 1, and an example of each operator family on a two-dimensional simplex element is given in Figure 1.

1. SBP- Ω Family

The SBP- Ω family, introduced in [18], contains nodes that are strictly on the interior of the element. Without constraining any of the nodes to lie on the boundary, more degrees of freedom exist in order to obtain a certain degree cubature rule to construct an SBP operator. Hence, either the number of points required to obtain a specific degree cubature rule will be minimized or the associated accuracy and degree will be maximized; this is analogous to an LG rule in one dimension. Therefore, the associated cubature rule will also produce an SBP operator that has a reduced solution L^2 norm error compared to the other SBP families [18]. However, because the nodes are in general not collocated with the boundary quadrature points, the projection operator R_j , and hence the directional surface integral E_{ξ} , is a dense matrix operator. Thus, the computation of the SATs can become more computationally intensive compared to the volume computations which use fewer points. The resultant efficiency of the SBP- Ω operators measured against these competing factors is not clear and is likely problem and implementation dependent.

2. SBP-F Family

The SBP- Γ family, introduced in [17], contains volume nodes that are in the interior of the element and at least $n_j \ge p + 1$ nodes on each facet of the element boundary for two-dimensional elements. Although the condition that $n_j \ge p + 1$ is not necessary, an SBP- Γ operator without this property will not take advantage of the more efficient projection operators that result. As some of the volume nodes are partially constrained to exist on the boundary facets, some of the degrees of freedom of the nodes are removed and hence the accuracy and degree of the cubature may be reduced or more points may be required to obtain a cubature rule of sufficient degree. This is analogous to an LGL rule in one dimension, where for *n* points, the LGL rule will produce a 2n - 3 quadrature rule as opposed to 2n - 1 for LG rules. Due to this, the associated SBP operator will either use more points than the SBP- Ω family for a given degree SBP operator, or for a given degree SBP operator and number of volume nodes *n*, the cubature rule and likely the SBP derivative operator will not be as accurate as one belonging to the SBP- Ω family. The benefit of using the SBP- Γ family is that the volume nodes that are constrained to exist on the boundary facets are collinear with the boundary cubature points. Thus, the computation of the SATs only requires the projection of those nodes which exist on the *j*th



Fig. 1 Examples of each SBP family of p = 2 multidimensional SBP operators constructed on a reference simplex element where (\circ) are the volume solution nodes and (\blacksquare) are the facet cubature points.

facet. This will reduce the number of arithmetic operations required to compute the SATs which may make the operator more efficient as the mesh is refined and the SAT computations become more dominant. However, the larger number of volume nodes and decreased accuracy for a specific degree SBP operator as compared to the SBP- Ω family can negate to a certain extent the efficiency obtained from more efficient SAT computations.

3. SBP-diag(E) Family

The SBP-diag(E) family, introduced in [29], contains nodes that are in the interior of the element and at least $n_j \ge p+1$ nodes on each facet of the element boundary that are collocated with the facet cubature points for two-dimensional elements. Similar to the SBP- Γ family, because some of the volume nodes are fully constrained to exist at the facet cubature points on the boundary facets, some of the degrees of freedom of the nodes are removed and hence the accuracy and degree of the cubature may be reduced or more points may be required to obtain a cubature rule of sufficient degree. Due to this, the associated SBP operator will either use more points than both the SBP- Ω and SBP- Γ families for a given degree SBP operator and number of volume nodes *n*, the cubature rule and likely the SBP operator will not be as accurate as the ones belonging to both the SBP- Ω and SBP- Γ families. The benefit of using the SBP-diag(E) family results from the collocation of the volume and facet cubature points. Due to this, no projection from the volume to the facet cubature points is required and the SATs can be computed directly in a point-wise and efficient fashion. As with the SBP- Γ family, the increased efficiency of the SAT computations may make these operators more efficient; however, it is not clear how the increased computational work due to an increase in the number of volume nodes will affect the overall efficiency of the SBP-diag(E) family.

IV. Symmetric and Positive Cubature Rules on Quadrilateral Elements

The search for symmetric and positive cubature rules in a specific canonical reference element is akin to the search for a multidimensional SBP operator. Various methods that possess the SBP property have utilized a tensor-product [11, 30– 34] node structure for the application to quadrilateral and hexahedral elements. Although optimal quadrature rules and interpolation points have been discovered in one dimension, namely the LG and LGL points, the extension of those rules through a tensor-product formalism in the construction of efficient and accurate SBP operators on quadrilateral elements may not necessarily produce the most efficient operators. This is primarily due to the additional symmetries and degrees of freedom that arise in dimensions greater than one which can be used to find more efficient and accurate cubature rules and hence SBP operators. We are concerned with the existence of truly multidimensional SBP operators on quadrilateral elements that can be used to construct SBP- Ω , SBP- Γ , and SBP-diag(E) families of operators. It is therefore worthwhile to understand the symmetry groups that exist in the quadrilateral element, as they will be used to construct the node sets for numerical optimization. We will consider the canonical quadrilateral reference element shown in Figure 2.

For the quadrilateral element, there exist four primary symmetry groups [27], with three additional auxiliary symmetry groups representing the restriction of the primary symmetry groups onto each face. The auxiliary symmetry groups are required to enforce the resultant SBP operator to belong to the SBP- Γ , and SBP-diag(E) families. The properties of each of these symmetry groups and cubature rules are contained in Table 2; they are also shown visually in Figure 3. The area of the reference quadrilateral is A = 4, which is used to normalize the cubature weights so that they sum to unity. Additionally, each symmetry group is associated with a single cubature weight.



Fig. 2 Canonical quadrilateral reference element.

Table 2	Properties of th	e symmetry	groups of a o	quaurnaterai.

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Symmetry Group	Number of Nodes	Node Position Parameters	# Node Position Parameters	# Cubature Weight Parameters
<i>s</i> ₁	1	(0,0)	0	1
<i>S</i> 41	4	$(\alpha, 0)$	1	1
s ₄₂	4	(α, α)	1	1
<i>s</i> ₈₁	8	(α, β)	2	1
s ₈₂	8	$(\alpha, 0)$	1	1
<i>S</i> 43	4	(0, 0)	0	1
<i>S</i> 44	4	(0, 0)	0	1

The search for cubature rules on the reference element, similar to the approach taken in [27], reduces to finding a set of points and weights which exactly integrates the tensor-product of an orthonormal basis of polynomials $\Phi_{ij} = \phi_i(x) \otimes \phi_j(y)$ of degree q, where i and j represent the degree of the polynomial such that $i + j \leq q$. By forming a linear combination of each of the symmetry groups, where each group except the s_1, s_{82}, s_{43} , and s_{44} groups have infinite multiplicity in the set of symmetry group decompositions, one can search for possible cubature rules by imposing the accuracy requirements of a degree q cubature rule. Knowing *a priori* if a certain number of points or a set of symmetry groups will form a valid cubature rule in order to construct an SBP operator is not obvious; thus, various numbers of nodes and symmetry group decompositions must be experimented with in order to find a valid cubature rule.

As an example, a valid cubature rule for an SBP- Γ family operator may involve the following linear combination of symmetry groups: $S = s_1 + s_{41} + s_{42} + s_{82}$. This set contains a total of 17 points, 3 free node location parameters, and 4 free weight parameters. The inclusion of the auxiliary symmetry group s_{82} is necessary in order to enforce a symmetric set of nodes to exist on the boundary of the element. One can also utilize the s_{43} and s_{44} groups; however, due to their unitary multiplicity, each group can only be included once. It would be desirable to include the s_{41} group if we wish to find an SBP-diag(E) family operator which utilizes LGL facet cubature points, since the collocation of the volume nodes with the corners would be necessary by definition. Regardless, in general, the inclusion of both the s_{43} and s_{44} groups is necessary, as the s_{82} group does not include the mid-edges or the corners.

The selection of the specific symmetry group decomposition is largely arbitrary, as long as the decomposition contains specific restrictions that satisfy the properties of the specific SBP family one is trying to generate. The algorithm utilized tests all symmetry group decompositions that satisfy the properties of the SBP family selected and also contain the desired number of nodes selected by the user.



Fig. 3 Symmetry groups of a quadrilateral including the auxiliary symmetry groups s_{82}, s_{43} , and s_{44} .

V. Summation-by-Parts Operator Accuracy Conditions

In addition to the symmetry groups chosen when constructing a multidimensional SBP operator, various conditions must be enforced to ensure that the operator has specific characteristics. These include the accuracy conditions of the cubature rule that the point set is associated with. The second condition is the degree of the SBP derivative operator, which must be exact for the set of degree p monomials restricted onto the point set \mathbf{p}_k . The third condition is the degree of the projection operator R_j , which must extrapolate the solution to the facet cubature points exactly for monomials of degree $r \ge p$. Together, these enforce the necessary accuracy conditions for a multidimensional SBP operator. For the studies presented in this paper, the facet cubature points will always be chosen as the degree p LG nodes, as they provide the most accurate quadrature with the minimum number of nodes. However, the choice of facet cubature points is arbitrary and various other points can be selected which may have preferential characteristics considered in this study.

A. Cubature Accuracy Conditions

The cubature accuracy conditions require that the cubature be of degree q, where $q \ge 2p - 1$ is necessary and sufficient for a degree p SBP operator [17]. Since the diagonal-norm matrix H is associated with the underlying cubature rule, the accuracy equations that the cubature rule with n nodes must satisfy are

$$\sum_{j=1}^{n} \mathsf{H}_{j,j} \mathcal{P}_{k}(\xi_{j}, \eta_{j}) = \int_{\Omega} \mathcal{P}_{k} d\Omega \quad \forall k \in \{1, 2, \dots, n_{q}^{*}\},$$
(3)

where $n_q^* = \binom{q+d}{d}$, and *d* is the dimension. This ensures that the resultant SBP operator possesses at least a degree 2p - 1 cubature rule.

B. Derivative Operator D_{ξ} Accuracy Conditions

Similarly, accuracy conditions can be imposed for the derivative operator D_{ξ} . The derivative operators in the other directions can be formed through a simple matrix permutation. Given that the derivative is a pointwise evaluation, we consider the Vandermonde matrix V which contains the restriction of the set of monomials onto the solution points $S_{\hat{\Omega}} = \{(\xi_i, \eta_i)\}_{i=1}^n$. The accuracy equations for a degree *p* SBP derivative operator can then be imposed in the ξ direction

$$\mathsf{D}_{\mathcal{E}}\mathsf{V}=\mathsf{V}_{\mathcal{E}},\tag{4}$$

$$\mathsf{H}^{-1}\mathsf{Q}_{\xi}\mathsf{V}=\mathsf{V}_{\xi},\qquad (\mathsf{D}_{\xi}=\mathsf{H}^{-1}\mathsf{Q}_{\xi})$$

$$\mathsf{Q}_{\xi}\mathsf{V} = \mathsf{H}\mathsf{V}_{\xi},\tag{5}$$

$$(\mathsf{S}_{\xi} + \frac{1}{2}\mathsf{E}_{\xi})\mathsf{V} = \mathsf{H}\mathsf{V}_{\xi}, \qquad (\mathsf{Q}_{\xi} = \mathsf{S}_{\xi} + \frac{1}{2}\mathsf{E}_{\xi})$$

$$S_{\xi}V = HV_{\xi} - \frac{1}{2}E_{\xi}V, \tag{6}$$

where V is of size *n* by n_p^* , and S_{ξ} is the skew-symmetric component of Q_{ξ} . By the skew-symmetry of S_{ξ} , there are a total of $n_{S_{\xi}} = \frac{n(n-1)}{2}$ undetermined parameters in S_{ξ} . These accuracy equations for the SBP derivative operator ensure that it is at least degree *p*.

C. Projection Operator R_i Accuracy Conditions

In order to ensure that the matrix operators can be decomposed into the associated bilinear forms present in the integration-by-parts formula, the projection operator R_j must satisfy specific accuracy constraints. For a quadrilateral, there are four distinct projection operators; however, because the node set is symmetric, the projection operator from the volume nodes to one facet and the projection operator of the volume nodes to another facet is a simple permutation of the columns of the operator. That is, if a projection operator is constructed on a reference facet denoted R_1 , and a matrix P is constructed which contains the permutation of the ordered node set in its columns, where P(:, 1) = 1 : n, then the other projection operators can be obtained as

$$R_j = R_1(:, P(:, j)), \quad j = 2, 3, 4.$$

Consider the volume Vandermonde matrix $V_{\hat{\Omega}}$ which contains the restriction of the set of monomials onto the volume solution points, and the facet Vandermonde matrix $V_{\hat{\Gamma}}$ which contains the restriction of the set of monomials onto the facet cubature points of a single reference facet for the canonical element. The accuracy equations are then imposed as

$$\mathsf{R}_1 \mathsf{V}_{\hat{\Omega}} = \mathsf{V}_{\hat{\Gamma}},\tag{7}$$

resulting in a set of linear equations to solve for the unknowns in R. In general, there are a total of $n \times n_f$ variables in R₁ which must be solved for, where *n* is the total number of volume nodes, and n_f is the total number of facet cubature points on a single facet. It is possible to exploit the symmetry of the operator to reduce the number of unknowns present in the equations, and such simplifications are used in the solution procedure described below.

VI. Procedure for Constructing Symbolic Summation-by-Parts Operators

In order to construct a degree p SBP operator on a given node set, the following procedure is performed:

- 1) Select the desired number of volume nodes *n* and decompose the nodes into potential symmetry orbits $S = \{S_i\}_{i=1}^k$.
- 2) For each symmetry group decomposition in *S*, solve the cubature accuracy equations in Eq. (3) to obtain a degree $q \ge 2p 1$ cubature rule with positive weights, that may or may not contain free parameters in the node positions and weights ω_i . Define H as H = diag(ω_i).
- 3) Define the projection operator R_j by solving the associated projection operator accuracy equations in Eq. (7) to obtain a projection operator that can exactly interpolate and extrapolate a polynomial of degree $r \ge p$. In this study, the degree r is chosen such that r = p.
- 4) Define the directional surface integral E_{ξ} using R_j and the associated decomposition given as $E_{\xi} = \sum_{j=1}^{n_{f_j}} R_j^T B_j N_{\xi j} R_j$.
- 5) Solve the set of linear derivative accuracy equations in Eq. (6) for the independent parameters in S_{ξ} .
- 6) Construct the associated derivative operator as $D_{\xi} = H^{-1}Q_{\xi}$, where $Q_{\xi} = S_{\xi} + \frac{1}{2}E_{\xi}$.
- 7) Optimize the *m* remaining free parameters for a specific objective $J(\mathbf{x})$, where $\mathbf{x} \in \mathbb{R}^m$, subject to specific constraints.
- 8) Construct the SBP operators in the remaining coordinate directions using the appropriate nodal permutations.

The above procedure is general in that it can be applied to SBP operators constructed in arbitrary dimensions and on arbitrary canonical reference elements such as triangles, quadrilaterals, tetrahedra, pyramids, prisms, and other unique polytopes.

VII. Numerical Optimization

Following the steps outlined above to construct a symbolic SBP operator, free parameters may remain which can serve as design variables in the numerical optimization of an SBP operator with respect to a specific objective function. This section will outline the design variables, objective functions, constraints, and the optimization strategy.

A. Design Variables

Suppose we decompose *n* points into a linear combination of symmetry groups *S*, which may form a cubature rule. This decomposition will be composed of n_p free node position parameters and n_w free cubature weight parameters. There are two methodologies for constructing and numerically optimizing an SBP operator:

- 1) Directly construct a degree q cubature rule by solving the nonlinear least-squares problem resulting from Eq. (3) for the symmetry group decomposition S and use the corresponding weights and nodal positions to solve Eq. (6) and Eq. (7).
- 2) Using the symmetry group decomposition *S*, solve Eqs. (3), (6) and (7), where the node positions and cubature weights may be free after satisfying the necessary accuracy conditions.

The first approach, similar to the methodologies in [27, 35], completely determines the cubature rule node positions and weights. Therefore, after numerically solving Eq. (3), the only free parameters that can serve as design variables in numerical optimization are those that remained undetermined in S_{ξ} and R_j . The second approach does not use a fully determined cubature rule in constructing the SBP operator, but rather uses the free parameters in the cubature rule after satisfying the degree conditions as the design variables, in addition to the free parameters that remained undetermined in S_{ξ} and R_j . The second approach is more general; however, the former approach is utilized in this paper as a preliminary investigation as we can efficiently construct a wide variety of SBP operators for various degrees while being confident that we are using a locally optimal cubature node set with a minimum norm of the cubature truncation error coefficients. However, due to the multi-modal and nonlinear nature of the cubature rule optimization problem, there is no guarantee that we have constructed a cubature rule that will have a globally optimal minimum norm of the cubature truncation error coefficients, or that this specific node set is optimal for the SBP operator optimization objective function.

B. Objective Functions

Various objective functions that influence computational efficiency can be used in the numerical optimization of an SBP operator. By computational efficiency we mean the ability to achieve a certain solution or functional error in a given amount of computational time. Properties affecting this include: the leading truncation error terms of the cubature rule and the SBP derivative operator, conditioning of the node set, the spectral radius of the derivative operator and equation specific system matrices, and dispersion and dissipation properties.

1. Norm of the Cubature Leading Truncation Error Coefficient

The cubature leading truncation error coefficient is the sum of the dominant error terms in the local Taylor expansion of the underlying SBP cubature rule. These error terms result when we apply a degree q cubature rule to a higher degree monomial for which the cubature rule is not exact. Additionally, we can take a linear combination of several higher degree error terms to minimize the first few truncation error terms. The cubature leading truncation error term and the objective function are defined as follows

$$\mathbf{e}_{k,\mathsf{H}}(i) = \sum_{j=1}^{n} \mathsf{H}_{j,j} \mathcal{P}_{k}(\xi_{j},\eta_{j}) - \int_{\Omega} \mathcal{P}_{k}(\xi_{j},\eta_{j}), \quad \forall k \in \{n_{p}^{*} + 1, n_{p}^{*} + 2, \dots, n_{i}^{*}\},$$
(8)

$$\mathcal{E}_{\mathsf{H},m} = \sum_{j=p+1}^{p+m} ||\mathbf{e}_{\mathsf{H}}(j)||, \quad m \ge 1,$$
(9)

where $||\cdot||$ is the standard L^2 norm. As the cubature rule is fully determined from the nonlinear least-squares optimization procedure, its parameters are fully determined prior to optimizing the SBP operator (as described in the first approach

given above). For a given orbit decomposition, we select a cubature rule with the smallest norm of the cubature truncation error coefficients and subsequently construct the SBP operator on this node set.

2. Norm of the Derivative Operator $D_{\mathcal{E}}$ Leading Truncation Error Coefficient

The derivative operator leading truncation error coefficient is the sum of the dominant error terms in the local Taylor expansion of the SBP derivative operator. These error terms result in a similar manner to the error terms that arise in the cubature rule. We can similarly take a linear combination of several higher degree error terms to minimize the first few truncation error terms as done in [20]. The derivative leading truncation error term and the objective function in the ξ direction are defined as follows

$$\mathbf{e}_{k,\mathsf{D}_{\xi}}(i) = \left\|\mathsf{D}_{\xi}\mathsf{V}_{:,k} - \mathsf{V}_{\xi_{:,k}}\right\|_{\mathsf{H}}, \quad \forall k \in \{n_p^* + 1, n_p^* + 2, \dots, n_i^*\},\tag{10}$$

$$\mathcal{E}_{\mathsf{D}_{\xi},m} = \sum_{j=p+1}^{p+m} ||\mathbf{e}_{\mathsf{D}_{\xi}}(j)||, \quad m \ge 1,$$
(11)

where $||\cdot||_{H}$ is the H-norm. Large magnitudes in the leading truncation error coefficient terms can have a negative effect in the asymptotic and pre-asymptotic convergence behaviour of the derivative operator, thereby decreasing its overall efficiency. Thus, it is desirable to minimize these terms in order to obtain a certain error threshold on a coarser mesh which will correspond to a more efficient operator.

3. Volume Node Vandermonde Condition Number

The volume node Vandermonde condition number is related to the interpolation accuracy of the point set and the ability to numerically compute the inverse of the volume node Vandermonde matrix. In the construction of the derivative operator D_{ξ} , and the projection operators R_j , we require the term $V_{\hat{\Omega}}^{-1}$. If our point set produces a Vandermonde matrix that has a high condition number and is therefore nearly singular, then an accurate numerical computation of the inverse will not be possible to machine precision. Demanding that our point set produce a low condition number will ensure that an accurate derivative and projection operator can be computed. The condition number of the volume Vandermonde matrix is represented as

$$C_{\mathsf{V}_{\hat{\Omega}}} = \operatorname{cond}(\mathsf{V}_{\hat{\Omega}}). \tag{12}$$

It is noted that the procedure in this paper selects a fully determined node set prior to the SBP operator numerical optimization procedure. For this reason, the condition number cannot be optimized and is merely used as a check to ensure that the selected cubature rule can produce an SBP operator that will not suffer from unwanted numerical issues.

4. Frobenius Norm

The Frobenius norm of the derivative operator provides an upper bound on its spectral radius such that $\rho(D_{\xi}) \leq ||D_{\xi}||_F$. The Frobenius norm of the derivative operator in the ξ direction is represented as

$$N_{\mathsf{D}_{\xi}} = ||\mathsf{D}_{\xi}||_F.$$
 (13)

One should expect that as the Frobenius norm increases, the spectral radius will also increase. Additionally, because the Frobenius norm is a convex function, it is simpler to optimize in comparison with the discontinuous behaviour of the spectral radius definition.

5. Spectral Radius

For linear conservation laws, after discretizing in space using the SBP derivative operator and applying the SATs, it is possible to write the resulting equations as

$$\frac{d\mathbf{u}}{dt} = \mathbf{R} = \mathbf{A}\mathbf{u} + \mathbf{f},\tag{14}$$

where **R** is the discrete residual, A is the Jacobian of the discrete residual, and **f** is a vector containing the SAT boundary conditions. For explicit time integration methods, the spectral radius of A, denoted as $\rho(A)$, provides an upper bound on

the maximum allowable time step for stability. That is

$$\Delta t \le \frac{C}{\rho(\mathsf{A})},\tag{15}$$

where *C* is a constant representing the stability region of the particular time integration method. Therefore, by minimizing the spectral radius of A, a larger stable time step can be taken which can lead to a more computationally efficient simulation - at least up to the point that the system becomes accuracy limited. Both the spectral radius of A and the spectral radius of the derivative operator D_{ξ} can be used as objective functions. These are represented as

$$S_{\mathsf{D}_{\mathcal{E}}} = \rho(\mathsf{D}_{\mathcal{E}}), \text{ and}$$
 (16)

$$S_{\mathsf{A}} = \rho(\mathsf{A}). \tag{17}$$

As A is the Jacobian for the entire discretization of the domain and is problem dependent, a surrogate matrix is utilized which represents the characteristic behaviour of the eigenvalues for the entire system matrix. The surrogate matrix for a single element on a periodic domain is defined as the derivative operator with the addition of a term representing an upwind numerical flux

$$\mathbf{A} = \mathbf{H}^{-1}(\mathbf{Q}_{\boldsymbol{\xi}} + \mathbf{R}_{1}^{\mathrm{T}}\mathbf{B}_{1}\mathbf{N}_{1}\mathbf{R}_{1}), \tag{18}$$

$$= \mathsf{D}_{\xi} + \mathsf{H}^{-1}\mathsf{R}_{1}^{\mathrm{T}}\mathsf{B}_{1}\mathsf{N}_{1}\mathsf{R}_{1}. \tag{19}$$

For the purposes of this investigation, the spectral radii of both D_{ξ} and A are recorded but not optimized. They serve as markers for when the operators experience numerical instability. In fact, it is found that the operators constructed with larger spectral radii require smaller time steps for stability, as expected.

6. Composite Objective Function

Various competing objective functions have been defined above that have nonlinear dependence on one another. In order to obtain an efficient operator that considers each of the objective functions, a composite objective function can be defined as follows:

$$J = \chi_1 \mathcal{E}_{\mathsf{H}} + \chi_2 \mathcal{E}_{\mathsf{D}_{\mathcal{E}}} + \chi_3 \mathcal{C}_{\mathsf{V}} + \chi_4 \mathcal{N}_{\mathsf{D}_{\mathcal{E}}} + \chi_5 \mathcal{S}_{\mathsf{D}_{\mathcal{E}}}, \tag{20}$$

$$\sum_{j} \chi_j = 1, \quad 0 \le \chi_j \le 1 \quad \forall j.$$
⁽²¹⁾

By selecting various values of χ , subject to the above conditions, a Pareto front can be generated in which various multidimensional SBP operators will form an optimal front relative to the objective functions used. This provides a family of operators that can be selected depending on which competing objectives are deemed more important than others for a specific application. The operators optimized in this investigation only use a single objective function so a Pareto front is not generated; this may be investigated in a future work.

C. Constraints

In addition to an objective function, we also require constraints to be imposed during the optimization to ensure the solution is a valid multidimensional SBP operator. The first of these constraints is that the cubature rule has positive weights; this is necessary to define a discrete norm for a diagonal-norm SBP operator. The second constraint is that the node positions are interior to the element. Although a valid SBP operator can be constructed with points exterior to the element, it is not a simple task to apply boundary conditions and therefore such solutions are not included in the multidimensional SBP operator optimization feasible region. Together these constraints are stated as:

$$H_{j,j} \ge 0$$
, for j = 1, 2, ..., n, and
 $|\xi_i| \le 1$, $|\eta_i| \le 1$, $\forall \xi_i, \eta_i \in S_{\hat{\Omega}} = \{(\xi_i, \eta_i)\}_{i=1}^n$

These constraints are not explicitly enforced in the numerical optimization of the SBP operators since a fully determined cubature rule is found in a separate nonlinear least-squares optimization routine prior to the optimization of the SBP operators. Instead, during the selection process of a valid cubature rule, these constraints are verified and are therefore satisfied automatically throughout the optimization of the SBP operator.

D. Optimization Strategy and Algorithms

Now that the objective functions and constraints have been established, the nonlinear numerical optimization problem is given as

 $\underset{\mathbf{x}}{\operatorname{arg min}} \quad J(\mathbf{x})$ subject to $\mathsf{H}_{j,j} \ge 0, \quad \text{for } \mathbf{j} = 1, 2, \dots, n, \text{ and}$ $|\xi_i| \le 1, \quad |\eta_i| \le 1, \quad \forall \xi_i, \eta_i \in S_{\hat{\Omega}} = \{(\xi_i, \eta_i)\}_{i=1}^n.$

Due to the nonlinear nature of the optimization problem and the multi-modal nature of the design space, we utilize MATLAB's Global Optimization package with the Sequential-Quadratic-Programming (SQP) method to optimize the design variables \mathbf{x} , subject to the constraints. Within the Global Optimization package we utilize the MultiStart optimization routine which generates random start points within the bounds of the constraints and distributes each point for parallel optimization using a local SQP solver. As a result of the variety of operators, parameters, and objective functions, the following naming convention is adopted to distinguish each optimized operator:

Family	The family of the SBP operator i.e. SBP- Ω , SBP- Γ , and SBP-diag(E),
n	the number of nodes in the discretization,
р	the degree of the SBP derivative operator,
q	the degree of the SBP cubature rule,
r	the degree of the SBP projection operator,
J	the objective function used in the optimization,
i	a unique cubature identifier for the operator.

VIII. Nonlinear Least-Squares Optimization of Cubature Rules

The process of selecting a valid node set to construct the SBP operator on is performed by solving a nonlinear least-squares optimization problem using an unconstrained Levenberg-Marquardt algorithm. Given *k* symmetry group decompositions, an iterative procedure is performed which attempts to minimize the squared error of the cubature approximation to the exact integration of a tensor-product of an orthonormal polynomial basis. Explicitly, given a symmetry group decomposition with *m* symmetry orbits containing *m* weights $\omega = \{\omega_1, \ldots, \omega_m\}$ and *m* sets of node parameters $(\alpha, \beta) = \{(\alpha, \beta)_1, \ldots, (\alpha, \beta)_m\}$:

For each $\{S_i\}_{i=1}^k$ symmetry group decomposition arg min $J(\mathbf{x})$, where $\mathbf{x} = \{\omega, (\alpha, \beta)\}$ $J(\mathbf{x}) = \sum_{i,j} \left(\sum_{l=1}^n \omega_{m(l)} \Phi_{ij}(x_l, y_l) - \int_{\hat{\Omega}} \Phi_{ij} d\hat{\Omega}\right)^2, \forall i + j \le q,$ $\Phi_{ij} = \phi_i \otimes \phi_j.$

This procedure is adopted from the optimization procedures performed in [27, 35] with modifications added to account for enforcement of the auxiliary groups required when considering the SBP- Γ and SBP-diag(E) families. Algorithm 1 was performed for cubature rules of degree $q \ge 2p - 1$ for p = 1, 2, 3, 4 and for the SBP- Ω , SBP- Γ , and SBP-diag(E) families. Table 3 contains the cubature rules that were successfully produced and were used in the subsequent construction of the multidimensional SBP operators on quadrilateral elements. Table 4 contains the properties of the cubature rules for the standard tensor-product LG and LGL nodes.

A. SBP-Ω Cubature Rules

The SBP- Ω cubature rules numerically derived and listed in Table 3 use fewer nodes for the same or lower degree LG and LGL tensor-product cubature rules listed in Table 4 and also possess a lower norm of the cubature truncation

	SBP-Ω														
Desired q	Obtained q	<i>s</i> ₁	<i>s</i> ₄₁	Orbit o	lecom	positio	on s43	s ₈₂	Nodes	# of Node Parameters	# of Weights	$\mathcal{E}_{\mathrm{H},1}$	$C_{V_{\hat{\Omega}}}$	Unique Identifier	Reference
	3	0	1	0	0	0	0	0	4	1	1	0.4619	1.0000	1	[27]
2	3	0	0	1	0	0	0	0	4	1	1	0.5028	1.0000	2	[27]
4	5	0	1	1	0	0	0	0	8	2	2	0.1402	2.1082	1	[27]
4	5	1	0	0	1	0	0	0	9	2	2	0.0954	1.7889	2	[*]
4	5	1	1	1	0	0	0	0	9	2	3	0.0934	2.4857	3	[*]
	7	0	1	2	0	0	0	0	12	3	3	0.0358	1.4807	1	[27]
	7	0	2	1	0	0	0	0	12	3	3	0.0662	2.7371	2	[27]
	7	1	1	0	1	0	0	0	13	3	3	0.0332	1.7936	3	[*]
	7	1	1	2	0	0	0	0	13	3	4	0.0251	1.8726	4	[*]
6	7	1	2	1	0	0	0	0	13	3	4	0.0681	2.7905	5	[*]
0	7	0	0	2	1	0	0	0	16	4	3	0.0322	2.0730	6	[*]
	7	0	1	1	1	0	0	0	16	4	3	0.0358	1.0472	7	[*]
	7	0	2	0	1	0	0	0	16	4	3	0.0302	2.7262	8	[*]
	7	0	2	2	0	0	0	0	16	4	4	0.0249	1.6649	9	[*]
	7	0	3	1	0	0	0	0	16	4	4	0.0664	2.8210	10	[*]
	9	0	1	2	1	0	0	0	20	5	4	0.0072	3.2601	1	[27]
	9	0	2	1	1	0	0	0	20	5	4	0.0071	3.2578	2	[27]
	9	1	0	1	2	0	0	0	21	5	4	0.0081	2.4786	3	[*]
	9	1	1	2	1	0	0	0	21	5	5	0.0055	2.6830	4	[*]
	9	1	2	1	1	0	0	0	21	5	5	0.0063	2.8185	5	[*]
8	9	0	0	2	2	0	0	0	24	6	4	0.0072	2.3301	6	[*]
	9	0	1	1	2	0	0	0	24	6	4	0.0031	2.9528	7	[*]
	9	0	1	3	1	0	0	0	24	6	5	0.0012	1.9556	8	[*]
	9	0	2	0	2	0	0	0	24	6	4	9.2628e-4	2.6009	9	[*]
	9	0	2	2	1	0	0	0	24	6	5	0.0038	1.8777	10	[*]
	9	0	3	1	1	0	0	0	24	6	5	0.0060	4.6228	11	[*]
									SB	Р-Г					
	1	0	0	0	0	0	0	1	8	1	1	0.9429	1.2248	1	[*]
2	3	1	0	0	0	0	0	1	9	1	2	0.4776	1.3021	2	[*]
_	3	0	0	1	0	0	0	1	12	2	2	0.0962	1.2025	3	[*]
	3	0	1	0	0	0	0	1	12	2	2	0.0813	1.3343	4	[*]
4	3	1	0	0	0	1	0	1	13	1	3	0.8060	4.2571	1	[*]
	5	0	0	1	0	1	0	1	16	2	3	0.1321	2.8457	2	[*]
	5	0	0	1	0	1	0	2	20	3	3	0.1324	3.3927	1	[*]
6	5	1	0	1	0	0	0	2	21	3	4	0.0742	3.5577	2	[*]
	7	0	1	1	0	0	0	2	24	4	4	0.0325	4.1800	3	[*]
	7	0	1	1	0	1	0	2	28	4	5	0.0363	5.2769	1	[*]
	7	1	0	0	1	1	0	2	29	4	5	0.0273	8.9790	2	[*]
8	7	1	1	1	0	1	0	2	29	4	6	0.0387	6.7280	3	[*]
	9	0	0	2	1	1	0	2	36	6	6	0.0081	4.2306	4	[*]
	9	0	1	1	1	1	0	2	36	6	6	0.0044	4.0799	5	[*]
	1		1	1					SBP-c	liag(E)		1		1	
	1	0	0	0	0	0	0	1	8	0	1	1.8856	1.4142	1	[*]
2	3	1	0	0	0	0	0	1	9	0	1	0.4929	1.3333	2	[*]
	3	0	0	1	0	0	0	1	12	1	2	0.0663	1.2301	3	[*]
	3	0	1	0	0	0	0	1	12	1	2	0.1082	1.2354	4	[*]
4	5	0	0	1	0	1	0	1	16	1	3	0.1321	2.8177	1	[*]
6	5	0	0	1	0	0	0	2	20	1	3	0.1528	4.0360	1	[*]
	7	0	1	1	0	0	0	2	24	3	4	0.0321	3.7759	2	[*]
	7	0	1	1	0	1	0	2	28	2	5	0.0363	5.9730	1	[*]
8	9	0	0	2	1	1	0	2	36	4	6	0.0088	5.9730	2	[*]
	9	0	1	1	1	1	0	2	36	4	6	0.0045	4.9682	3	[*]

Table 3Properties of the valid cubature rules constructed using Algorithm 1, potentiallynew cubature rules are indicated with a star [*].

Algorithm 1 Algorithm used for the nonlinear optimization of cubature rules.

- 1) Select the desired SBP operator and populate the required auxiliary symmetry orbit decompositions, use the remaining nodes to populate the primary symmetry groups
- 2) Seed an initial random guess for the node position parameters
- 3) For each Φ_{ij} , evaluate $b_k = \int_{\hat{\Omega}} \Phi_{ij} d\hat{\Omega}$
- 4) Construct a matrix A ∈ ℝ^{k×m⁻} which contains the evaluation of the cubature weighted sum of the tensor-product orthonormal polynomials at each node *n* (columns) in symmetry orbit *m* and for each degree in each row i.e. A_{km} = ∑_m ∑_{n∈m} Φ_k(x_n, y_n)
- 5) Solve for the weights by solving the linear system $A\omega = b$
- 6) Evaluate the objective function $J(\mathbf{x}) = \|\mathbf{r}\|$, where $\mathbf{r} = A\omega b$
- 7) Perform a Levenberg-Marquardt solution update
- 8) Repeat steps 3-7 to convergence i.e. $\|\mathbf{r}\| \le \epsilon$, where ϵ is a tolerance representing machine precision
- 9) Eliminate any rules which are exterior to the canonical domain and contain negative weights
- 10) Eliminate the cubature rules with a Vandermonde condition number that is not on the order of unity, and of the cubature rules remaining, choose the rule with the smallest norm of the cubature truncation error coefficient.

	Tensor	-Product	Legendre-Gauss				
q	Nodes	$\mathcal{E}_{H,1}$	$cond(V_{\hat{\Omega}})$				
3	4	0.5028	1.0000				
5	9	0.1293	1.4512				
7	16	0.0328	1.6796				
9	25	0.0083	2.1434				
Te	nsor-Pro	duct Lege	endre-Gauss-Lobatto				
1	4	3.7712	1.7320				
3	9	0.7542	3.5098				
5	16	0.1724	3.9679				
7	25	0.0410	5.2749				

Table 4Properties of the tensor-product cubature rules.

error coefficients. It has been identified previously that accurate cubature rules seem to produce SBP operators with preferential error properties [18]. This appears to indicate that these new cubature rules have the potential to have better solution accuracy when compared to tensor-product operators. The relative conditioning of the volume Vandermonde matrix also maintains a value on the order of unity, and is approximately the same magnitude of the tensor-product nodal distributions. This indicates that the node set is well behaved for spatial discretization.

B. SBP-Г Cubature Rules

The SBP- Γ cubature rules use more nodes in general than the tensor-product LG and LGL operators of equal degree. As we demand the exact integration of a 2*p* polynomial on the facets of the quadrilateral, we force a minimum of 4(p+1) nodes on the boundaries so that we can maintain the sparse interpolation properties of the R_j projection operator. However, despite the fact that we must restrict these nodes onto the facets of the quadrilateral, the use of additional nodes also allows us to maintain a relatively low cubature truncation error. For all degree *q* cubature rules, we were able to produce a cubature rule with a smaller norm of the cubature truncation error coefficients than the LGL nodal distribution. In some cases the norm of the cubature truncation error coefficients is also better than the LG nodes for the equivalent cubature degree. The condition number of the volume Vandermonde matrix was also maintained on the order of unity, indicating that the cubature rules constructed have preferential interpolation properties. However, it is emphasized again that these improvements were obtained by increasing the number of nodes compared to the tensor-product cubature rules.

	Tensor-Product Legendre-Gauss											
p	Name	n	q	r	NNZ _D	$\mathcal{E}_{D_{\xi},1}$	$\mathcal{E}_{D_{\xi},2}$	$\mathcal{N}_{D_{\xi}}$	$\mathcal{S}_{D_{\xi}}$	\mathcal{S}_{A}		
1	LG[4,1,3,1]_()_1	4	3	1	8	5.3333	5.8962	2.4498	0	2.5811		
2	LG[9,2,5,2]_()_1	9	5	2	24	3.8400	4.4800	8.2158	1.3939e-5	6.1590		
3	LG[16,3,7,3]_()_1	16	7	3	64	2.0898	2.5347	18.4390	3.8494e-4	11.1957		
4	LG[25,4,9,4]_()_1	25	9	4	120	0.9675	1.2067	34.0347	0.0032	17.6813		
			Ten	sor-	Product L	egendre-G	auss-Loba	tto				
1	LGL[4,1,1,-]_()_1	4	1	-	8	16.0000	27.7128	1.4142	0	1.3660		
2	LGL[9,2,3,-]_()_1	9	3	-	24	8.0000	9.9778	6.3639	1.0607e-5	4.2311		
3	LGL[16,3,5,-]_()_1	16	5	-	56	3.4133	4.1400	15.4919	3.2652e-4	8.5512		
4	LGL[25,4,7,-]_()_1	25	7	-	110	1.3061	1.5661	29.5237	0.0022	14.3182		

 Table 5
 Properties of the SBP operators constructed on tensor-product cubature rules.

C. SBP-diag(E) Cubature Rules

Similar to the SBP- Γ cubature rules, the SBP-diag(E) cubature rules use more nodes than tensor-product LG and LGL nodes of equal degree. Since we wish to obtain a diagonal-E operator (i.e. collocation with the facet cubature points) and the exact integration of a degree 2*p* polynomial on the facets of the quadrilateral, we force a minimum of 4(p + 1) nodes on the boundaries. The benefit is the construction of SBP operators that have very efficient interelement coupling in comparison to the SBP- Γ and SBP- Ω operators. The obtained cubature rules show a smaller norm of the cubature truncation error coefficients compared to the LGL tensor-product nodes for equivalent cubature degrees. For some cases, the norm of the cubature truncation error coefficients was also lower than the tensor-product LG cubature rule; however, the significant increase in the number of required nodes may outweigh the added efficiency from the collocation with the facet cubature points and the lower norm of the cubature truncation error coefficients.

Despite the clear improvements in the cubature rules obtained over the tensor-product cubature rules, it is necessary to perform numerical experiments testing the constructed SBP operators on the non-tensor-product nodal distributions in comparison to the tensor-product nodal distributions due to many competing factors in the discretization of partial differential equations. Figures showing the nodal distributions for some of the operators in Table 3 are given in the Appendix.

IX. Numerical Optimization of Summation-by-Parts Free Parameters

Once the cubature rules were obtained, the procedure outlined in Section VI was followed to produce symbolic SBP operators with free parameters in the undetermined matrix operators. As H and the associated node set $S_{\hat{\Omega}}$ is fully determined from the cubature rule, the possible free parameters which can be optimized result from constructing R_j and S_{ξ} . The properties of the SBP operators constructed on the LG and LGL tensor-product nodal distributions are given in Table 5

The free parameters that remained after constructing the SBP operators in the numerically optimized cubature rules in Table 3 were optimized for the norm of the first two leading truncation error terms in the derivative operator D_{ξ} . That is, the nonlinear optimization problem given in Section VII.D was solved with the outlined procedure with

$$J(\mathbf{x}) = \mathcal{E}_{\mathsf{D}_{\mathcal{E}},2}$$

It has been found that this objective function also correlates with the spectral radius of the derivative operator [9]; therefore, operators that are optimized for reduced derivative truncation error tend to also reduce the spectral radius of the derivative matrix operator (and by extension, the system matrix A) [20, 21].

	SBP-Ω													
	р	Name	n	q	r	No. FP R_j	No. FP S_{ξ}	No. FP	$NNZ_{D_{\xi}}$	$\mathcal{E}_{D_{\mathcal{E}},1}$	$\mathcal{E}_{D_{\xi},2}$	$N_{D_{\xi}}$	$\mathcal{S}_{D_{\xi}}$	SA
Γ	1	SBP-Ω[4,1,3,1]_E _{Dξ,2} 1	4	3	1	1	0	1	16	5.3333	5.8962	2.4495	0	2.5812
	1	SBP- $\Omega[4,1,3,1]_{\mathcal{E}_{D_{\xi},2}}^{2}$	4	3	1	1	0	1	12	2.3094	5.0869	2.4495	1.4443e-6	3.4845
Γ		SBP-Ω[8,2,5,2]_E _{Dξ,2} 1	8	5	2	3	1	4	60	2.6808	3.9212	7.1701	1.9210e-4	7.1006
	2	SBP-Ω[9,2,5,2]_E _{Dξ,2} _2	9	5	2	4	3	7	80	1.6111	2.5800	8.1813	0.3570	8.5606
		SBP-Ω[9,2,5,2]_E _{Dξ,2} _3	9	5	2	5	3	8	78	1.4962	1.9319	8.2628	0.0020	9.9123
		SBP-Ω[12,3,7,3]_E _{Dξ,2} _1	12	7	3	4	1	5	140	1.4494	2.0099	14.1146	0.0015	12.6223
		SBP- $\Omega[12,3,7,3]_{\mathcal{E}_{D_{\xi},2}}^{2}$	12	7	3	4	1	5	136	1.3494	2.2646	12.6247	0.0029	13.0938
		SBP-Ω[13,3,7,3]_ <i>E</i> _{D_ξ,2_} 3	13	7	3	6	3	9	164	0.6530	1.4826	18.3339	0.0025	59.2771
		SBP- $\Omega[13,3,7,3]_{\mathcal{E}_{D_{\xi},2}}4$	13	7	3	6	3	9	164	0.8837	1.5883	14.8087	0.0013	13.2734
	2	SBP- $\Omega[13,3,7,3]_{\mathcal{E}_{D_{\xi},2},5}$	13	7	3	6	3	9	160	1.2833	2.2646	18.5231	0.0148	1.2279e+2
	3	SBP-Ω[16,3,7,3]_ <i>E</i> _{D_ξ,2} _6	16	7	3	12	15	27	256	1.6406	2.0043	90.0243	1.9689	5.2490e+3
		SBP- $\Omega[16,3,7,3]_{\mathcal{E}_{D_{\xi},2}}^{-7}$	16	7	3	12	15	27	254	0.5478	1.0389	3.4009e+2	1.9183	8.5449e+3
		SBP-Ω[16,3,7,3]_ <i>E</i> _{D_ξ,2} _8	16	7	3	12	15	27	252	0.6587	1.0432	24.0229	1.6218	41.1286
		SBP-Ω[16,3,7,3]_ <i>E</i> _{D_ξ,2} _9	16	7	3	12	15	27	252	0.4976	1.0435	31.0858	1.1415	35.0998
		SBP- Ω [16,3,7,3]_ $\mathcal{E}_{D_{\xi},2}$ _10	16	7	3	12	15	27	250	1.3505	1.7917	4.3756e+2	2.8564	7.7349e+2
		SBP-Ω[20,4,9,4]_E _{Dξ,2} _1	20	9	4	12	10	22	396	0.4353	0.7314	27.7650	0.9854	21.6165
		SBP- $\Omega[20,4,9,4]_{\mathcal{E}_{D_{\xi}},2}^{-2}$	20	9	4	13	10	23	396	0.4220	0.6632	27.3160	0.4615	23.6000
		SBP-Ω[21,4,9,4]_ <i>E</i> _{D_ξ,2_} 3	21	9	4	14	15	29	440	0.3078	0.6097	32.7052	3.4758	29.2618
		SBP- $\Omega[21,4,9,4]_{\mathcal{E}_{D_{\xi}},2_{4}}$	21	9	4	15	15	30	438	0.3290	0.4886	28.8801	0.9142	25.5389
		SBP- $\Omega[21,4,9,4]_{\mathcal{E}_{D_{\xi}},2_{5}}$	21	9	4	16	15	31	436	0.3475	0.5532	32.2869	1.2681	80.7609
	4	SBP- $\Omega[24,4,9,4]_{\mathcal{E}_{D_{\xi},2}}6$	24	9	4	21	35	57	576	0.0432	0.5517	6.9451e+2	8.6601	4.6538e+3
		SBP-Ω[24,4,9,4]_E _{D_ξ,2_7}	24	9	4	22	36	58	574	0.0136	0.2902	35.0379	1.7221	31.0888
		SBP-Ω[24,4,9,4]_E _{Dξ,2} _8	24	9	4	22	36	58	574	0.0040	0.2736	40.8412	1.9018	27.8969
		SBP- $\Omega[24,4,9,4]_{\mathcal{E}_{D_{\xi},2}}9$	24	9	4	23	36	59	572	0.0033	0.2127	32.2738	1.3747	26.9012
		SBP- $\Omega[24,4,9,4]_{\mathcal{E}_{D_{\xi},2}}$ 10	24	9	4	23	36	59	572	0.0069	0.2857	43.5747	1.4145	43.5037
		SBP-Ω[24,4,9,4]_ <i>E</i> _{D_ξ,2} _11	24	9	4	24	36	60	570	0.0305	0.3704	46.9708	2.5023	1.8260e+2

Table 6 Properties of the optimized SBP operators constructed on the numerically optimized SBP- Ω cubature nodes. No. FP indicates the number of free parameters in the respective matrix operator.

A. Norm of the First Two Leading Derivative Truncation Error Coefficients

1. SBP- Ω Operators

Using the numerically optimized SBP- Ω cubature nodes, SBP- Ω operators were constructed and the free parameters were optimized to minimize the norm of the first two truncation error coefficients of the derivative operator. The properties of the operators are contained in Table 6. It is clear that the optimization procedure was successful in that we were able to obtain SBP- Ω operators with smaller derivative truncation terms than the LG and LGL tensor-product nodal distributions. One would expect that this would improve the accuracy of the derivative approximation. However, because our nodal distribution is fully coupled, our derivative matrix operator is dense, in contrast to the sparse diagonal structure of the tensor-product nodal distributions. As a result, it has a greater number of number of nonzeros (NNZ) than a tensor-product operator. This increases the computational cost of these operators and is measured by the NNZ_{D_ξ} column. Also, due to the fully coupled structure of these operators we also have a dense projection operator R_j, which increases the cost of the quadrature facet integration. Additionally, we see that the spectral radius of the derivative operator and the associated system matrix is significantly larger than the tensor-product nodal distributions. As a result, it may be beneficial to optimize the free parameters in the SBP operator with a composite objective function which includes a linear combination of the norm of the derivative truncation error coefficients and the spectral radius of the derivative truncation error coefficients and the spectral radius of the derivative truncation error coefficients and the spectral radius of the derivative truncation error coefficients and the spectral radius of the derivative truncation error coefficients and the spectral radius of the derivative truncation error coefficients and the spectral radius of the derivative truncation error coefficients and the spectral radius of the derivative truncation error coefficients and the spectral radi

2. SBP-T Operators

Using the same objective function, the SBP- Γ operators were constructed on the numerically optimized SBP- Γ node sets. The properties of these operators are contained in Table 7. The purpose of constructing SBP- Γ operators is to take advantage of having more degrees of freedom than the SBP-diag(E) family to obtain a potentially more accurate SBP operator while also maintaining a relatively sparse projection operator. These two competing factors play

	SBP-Г												
p	Name	п	q	r	No. FP R_j	No. FP S_{ξ}	No. FP	NNZ _D	$\mathcal{E}_{D_{\xi},1}$	$\mathcal{E}_{D_{\xi},2}$	$N_{D_{\xi}}$	$\mathcal{S}_{D_{\mathcal{E}}}$	SA
	SBP-Γ[8,1,1,1]_ $\mathcal{E}_{D_{\xi},2}$ _1	8	1	1	0	10	10	60	1.0379e+4	1.7877e+4	2.1951e+4	1.5521e+4	4.6563e+4
1	SBP-Γ[9,1,3,1]_ <i>E</i> _{D_ξ,2} _2	9	3	1	0	15	15	76	1.0166	3.1713	7.0570	1.8916	6.7387
1	SBP-Γ[12,1,3,1]_ $\mathcal{E}_{D_{\xi},2}_{-3}$	12	3	1	0	36	36	136	0.2710	0.4161	1.1235e+2	55.2531	54.7096
	SBP-Γ[12,1,3,1]_ <i>E</i> _{D_ξ,2_4}	12	3	1	0	36	36	136	0.7445	1.1951	1.4899e+2	88.0558	87.6834
2	SBP-Γ[13,2,3,2]_& _{D_ξ,2_1}	13	3	2	0	21	21	162	80.9947	96.1832	5.4355e+2	2.6686e+2	8.8821e+2
1	SBP- Γ [16,2,5,2]_ $\mathcal{E}_{D_{\xi},2}$ _2	16	5	2	0	45	45	246	0.6668	1.7636	4.5172e+2	2.8131e+2	2.8122e+2
	SBP-Γ[20,3,5,3]_E _{D_ξ,2_1}	20	5	3	0	45	45	388	2.5572	15.2474	1.4524e+3	9.5545e+2	2.9572e+3
3	SBP-Γ[21,3,5,3]_ <i>E</i> _{D_ξ,2} _2	21	7	3	0	55	55	428	0.9848	1.6416	4.7173e+2	2.5636e+2	2.5594e+2
	SBP-Γ[24,3,7,3]_ <i>E</i> _{D_ξ,2_} 3	24	7	3	0	91	91	560	0.5251	0.9808	77.2015	9.7649	43.8297
	SBP-Γ[28,4,7,4]_ <i>E</i> _{D_ξ,2_} 1	28	7	4	0	78	78	766	3.5013	4.0035	2.7269e+2	25.6449	3.0099e+2
	SBP-Γ[29,4,7,4]_ <i>E</i> _{D_ξ,2} _2	29	7	4	0	91	91	822	0.8780	1.2011	6.9590e+3	4.9114e+3	4.9112e+3
4	SBP-Γ[29,4,7,4]_ <i>E</i> _{D_ξ,2_} 3	29	7	4	0	91	91	822	1.0954	1.3163	1.5785e+2	18.5491	1.7278e+2
	SBP-Γ[36,4,9,4]_ <i>E</i> _{D_ξ,2} _4	36	9	4	0	210	210	1270	0.1178	0.3201	7.5029e+3	8.9749e+2	1.8398e+3
	SBP-Γ[36,4,9,4]_ <i>E</i> _{D_ξ,2_5}	36	9	4	0	210	210	1270	0.3475	0.5532	32.2869	1.2681	80.7609

Table 7 Properties of the optimized SBP operators constructed on the numerically optimized SBP- Γ cubature nodes. No. FP indicates the number of free parameters in the respective matrix operator.

critical roles in the overall efficiency of the discretization. In order to allow for exact integration of the facet cubature points, significantly more nodes are required as compared to the tensor-product LG and LGL nodes. This introduces a large number of free parameters in S_{ξ} which can be optimized. For all cases, no free parameters were available for optimization in R_j . This is because, for two dimensions, there are always p + 1 unknowns in R_j for the SBP- Γ family, and since we demand p + 1 nodes are present on the facet, this results in p + 1 independent equations. This system has a unique solution and is therefore fully determined.

For all degrees, our optimization procedure was able to obtain SBP- Γ operators with significantly lower norms of the first and second derivative truncation error coefficients. However, this was largely at the expense of either coupling all of the nodes together, using more nodes than the tensor-product nodal distributions, and also having a significantly larger spectral radius for D_{ξ} and A. Furthermore, it appears that the large order of magnitude increase in the spectral radius of some of the derived operators may render them impractical for explicit time integration methods. It is not clear if this will play a significant impact for implicit time integration methods; however, the dense structure and the spectral radius could negatively affect overall conditioning of the linearized system.

3. SBP-diag(E) Operators

Using the same procedure as the previous two families of SBP operators, the operators in the SBP-diag(E) family were optimized on their corresponding node sets. The results of this optimization are contained in Table 8. The SBP-diag(E) family provides the most efficient computation of the SAT coupling at the facet cubature points. This increase in efficiency results from sacrificing the ability to move the nodes restricted onto the facets for interpolation. That is, 4(p + 1) nodes are fully determined and their only degree of freedom which contributes to the overall properties of the operator is the cubature weight associated with the symmetry group. It is therefore expected that these operators will have inferior accuracy properties to the SBP- Ω and SBP- Γ families. As we also require collocation with the 4(p + 1) quadrature points, the SBP-diag(E) operators tend to have more nodes than the equivalent degree LG and LGL tensor-product SBP operators. As a result, there exist many free parameters in S_{\varepsilon} that can be optimized for our specific objective function. Similar to the SBP- Γ operators, these free parameters are strictly from S_{\varepsilon}, since R_j is fully determined from the facet collocation.

For each degree, we were again able to significantly reduce the norm of the derivative truncation error terms in comparison to the SBP operators constructed on tensor-product LG and LGL nodal distributions. However, this was again at the expense of coupling the degrees of freedom, therefore significantly increasing the number of nonzeros in D_{ξ} , and increasing the spectral radius of D_{ξ} and the associated system matrix A. An SBP operator constructed on the LGL nodes represents a tensor-product equivalent of the SBP-diag(E) family. The LGL nodes are however incapable of obtaining a degree 2p facet cubature and therefore do not integrate the SAT penalty terms exactly. Having exact integration of these terms is important in constructing entropy-stable schemes. Therefore, the novel SBP-diag(E) operators derived here which have $q \ge 2p$ volume cubature degree and q = 2p facet cubature degree can have potential

Table 8Properties of the optimized SBP operators constructed on the numerically
optimized SBP-diag(E) cubature nodes. No. FP indicates the number of free parameters
in the respective matrix operator.

	SBP-diag(E)												
p	Name	n	q	r	No. FP R_j	No. FP S_{ξ}	No. FP	$NNZ_{D_{\mathcal{E}}}$	$\mathcal{E}_{D_{\xi},1}$	$\mathcal{E}_{D_{\xi},2}$	$N_{D_{\xi}}$	$S_{D_{\xi}}$	SA
	SBP-diag(E)[8,1,1,1]_ $\mathcal{E}_{D_{\xi},2}_{1}$	8	1	1	0	10	10	60	6.5993	8.8695	3.6793	1.2501	2.7075
1	SBP-diag(E)[9,1,3,1]_ $\mathcal{E}_{D_{\xi},2}_{2}$	9	3	1	0	15	15	76	0.8238	3.1940	7.0330	1.8350	5.7095
1	SBP-diag(E)[12,1,3,1]_ $\mathcal{E}_{D_{\xi},2}$ _3	12	3	1	0	36	36	136	0.1524	0.2751	79.3877	38.7521	38.4958
	SBP-diag(E)[12,1,3,1]_ $\mathcal{E}_{D_{\xi},2}_4$	12	3	1	0	36	36	136	0.2242	0.4014	2.1102e+2	1.1103e+2	1.1102e+2
2	SBP-diag(E)[16,2,5,2]_ $\mathcal{E}_{D_{\xi},2}$ _1	16	5	2	0	45	45	246	0.6758	1.7653	7.7633e+2	4.8413e+2	4.8408e+2
3	SBP-diag(E)[20,3,5,3]_ $\mathcal{E}_{D_{\xi},2}$ _1	20	5	3	0	45	45	388	2.8709	3.3750	19.7998	2.7762	13.3585
	SBP-diag(E)[24,3,7,3]_ $\mathcal{E}_{D_{\xi},2}$ _2	24	7	3	0	91	91	560	0.7295	1.2187	1.0709e+2	13.9612	78.5137
	SBP-diag(E)[28,4,7,4]_ $\mathcal{E}_{D_{\xi},2}$ _2	28	7	4	0	78	78	766	1.6427	1.7547	86.2597	6.2836	52.2252
4	SBP-diag(E)[36,4,9,4]_ $\mathcal{E}_{D_{\xi},2}_{4}$	36	9	4	0	210	210	1270	0.1055	0.3291	62.2726	13.2130	30.9556
	SBP-diag(E)[36,4,9,4]_ $\mathcal{E}_{D_{\xi},2}$ 5	36	9	4	0	210	210	1270	0.0678	0.1253	97.1795	23.2367	45.5275

benefits within this context.

X. Numerical Experiments

The numerical experiments presented aim to compare the relative accuracy and efficiency of these newly developed non-tensor-product SBP operators on quadrilateral elements in comparison to equal degree tensor-product SBP operators on LG and LGL nodes. These experiments investigate the relative accuracy and efficiency for both linear (linear advection) and nonlinear (Euler equations) equations for canonical test problems. The experiments were performed on both uniform and curvilinear meshes but only the latter results are presented as the general trends were the same.

One advantage of the tensor-product structure is that it significantly increases the sparsity of the derivative operator. In addition, because of the tensor-product structure, the operator exactly differentiates the complete tensor-product monomial basis and therefore the leading monomial truncation error terms that are not high degree along the ξ or η directions, i.e. the derivative of the terms of the form

$$\xi^i \eta^j, \quad \forall i+j < p+1, \quad i,j < p+1$$

are automatically exact. As an example, a p = 1 non-tensor-product operator will exactly differentiate the monomials 1, ξ , and η . However, an equal degree tensor-product operator will in addition exactly differentiate the "bilinear" monomial $\xi\eta$. The sparsity structure of the LG and LGL nodes is not fully taken advantage in the residual computations; therefore, the cost comparison given here may be introducing unnecessary multiplications with 0 entries in the derivative matrix.

A. Two-Dimensional Linear Advection Equation: Gaussian Pulse

1. Problem Definition

For the linear case, we consider the advection of a compactly supported (to machine precision) Gaussian pulse on a curvilinear periodic domain. The linear advection equation in strong conservation form is given as

$$\frac{\partial \mathcal{U}}{\partial t} + a_x \frac{\partial \mathcal{U}}{\partial x} + a_y \frac{\partial \mathcal{U}}{\partial y} = 0,$$
(22)

with the initial condition,

$$\mathcal{U}(x, y, 0) = \exp\left(\frac{-(x-\mu)^2}{2\sigma^2}\right) \exp\left(\frac{-(y-\mu)^2}{2\sigma^2}\right),$$

$$\mu = 0.5,$$

$$\sigma = 0.1.$$

The wave speeds in the x and y directions are $a_x = 0.5$ and $a_y = 0.5$, respectively. Furthermore, we consider a periodic domain defined on $\Omega \in [0 \ 1] \times [0 \ 1]$ and the time domain $t \in [0 \ 2]$. Fig. 5 contains the coarsest grid used in this



Fig. 4 The second coarsest curvilinear grid level used on the domain $[0\ 1] \times [0\ 1]$ with 20×20 total elements.

numerical simulation. The associated curvilinear transformation is given as

$$x = \xi + \alpha \cos(\pi(\xi - 0.5)) \cos(\pi(\eta - 0.5)),$$

$$y = \eta + \alpha \cos(\pi(\xi - 0.5)) \cos(\pi(\eta - 0.5)),$$

where $\alpha = 1/8$. After discretizing the spatial derivatives with SBP operators, the semi-discrete system is integrated in time using 4th-order Runge-Kutta time integration with a constant CFL of 0.01. Additionally, we utilize upwind numerical fluxes in the computation of the SAT coupling terms to add sufficient dissipation to stabilize the problem and to obtain optimal orders of convergence.

For the convergence results, five grid levels were constructed resulting in a total of [100 400 900 1600 2500] elements on each level. At each grid level, the norm of the solution error and the CPU time in seconds was recorded, as presented in the following sections.

2. Solution Error Results

The comparison of the H-norm $(|| \cdot ||_{H})$ of the solution error for SBP operators constructed on tensor-product LG and LGL nodes and the new non-tensor-product SBP operators on quadrilateral elements are contained in Fig. 5. Candidate SBP operators that require prohibitively small time steps with the 4th-order Runge-Kutta method are not shown. For the p = 1 case, the SBP- $\Omega[4,1,3,1]_{\mathcal{E}_{De,2}}$ operator is exactly the same as the LG p = 1 operator, therefore producing identical error properties. Most of the SBP-diag(E) operators for each degree can achieve better solution error than the LGL operator, which indicates that they may be beneficial in entropy-stable schemes where facet cubature collocation is desirable for improved efficiency. The SBP- Ω operators achieve roughly the same error as the LG operators for all degrees with fewer volume nodes; however, this is at the expense of fully coupling the node set. It may be beneficial to increase the number of volume nodes of the SBP- Ω operators to equal that of the LG nodes for a given degree to see if the additional degrees of freedom allow for the construction of a more accurate SBP operator. The SBP- Γ operators generally have accuracy between the SBP- Ω and SBP-diag(E) operators as expected. For the p = 1 case, the large number of nodes of the SBP-diag(E) and SBP- Γ allow enough freedom to achieve operators with better accuracy than both the LG and LGL nodes. Design order of convergence is generally achieved, and the experimental rates of convergence for each of these operators is given in Table 9. Exceptions to this are cases of the SBP- Γ and SBP-diag(E) operators which appear to underconverge for each order. For the p = 4 cases, the experimental orders of convergence fall slightly below the expected value of p + 1 = 5, which may be due to the influence of time integration error as the spatial error is relatively small on the finer meshes.

p = 1		<i>p</i> = 2				
Name	Rate	Name	Rate			
LG $p = 1$	2.4767	LG $p = 2$	3.3631			
LGL $p = 1$	1.2270	LGL $p = 2$	3.3565			
SBP- $\Omega[4, 1, 3, 1]_{\mathcal{E}_{D_{\xi}, 2}}$	2.6686	SBP- $\Omega[8, 2, 5, 2] \mathcal{E}_{D_{\xi}, 2} 1$	3.0844			
SBP- $\Omega[4, 1, 3, 1]_{\mathcal{E}_{D_{\xi}, 2}}^2$	2.7515	SBP- $\Omega[9, 2, 5, 2]_{\mathcal{E}_{D_{\xi}, 2}}^{2}$	3.2117			
SBP- $\Gamma[9, 1, 3, 1] _ \mathcal{E}_{D_{\xi}, 2} _ 2$	2.4024	SBP- $\Omega[9, 2, 5, 2] \mathcal{E}_{D_{\xi}, 2} 3$	3.1970			
SBP- $\Gamma[12, 1, 3, 1] \mathcal{E}_{D_{\xi}, 2} 3$	1.6455	SBP- $\Gamma[16, 2, 5, 2] \mathcal{E}_{D_{\xi}, 2} 2$	2.9921			
SBP-diag(E)[8, 1, 1, 1]_ $\mathcal{E}_{D_{\xi}, 2}$ _1	1.6918	SBP-diag(E)[16, 2, 5, 2]_ $\mathcal{E}_{D_{\xi}, 2}$ _1	2.9926			
SBP-diag(E)[9, 1, 3, 1]_ $\mathcal{E}_{D_{\xi}, 2}_{2}$	2.4887	-	-			
SBP-diag(E)[12, 1, 3, 1]_ $\mathcal{E}_{D_{\xi}, 2}$ _3	1.5913	-	-			
<i>p</i> = 3		<i>p</i> = 4				
Name	Rate	Name	Rate			
LG $p = 3$	4.1240	LG $p = 4$	4.0834			
LGL $p = 3$	4.1448	LGL $p = 4$	4.7547			
SBP- $\Omega[12, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}}$	4.0148	SBP- $\Omega[20, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} $	4.6777			
SBP- $\Omega[12, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}}^{2}$	4.0256	SBP- $\Omega[20, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} \$	4.6990			
SBP- $\Omega[13, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}_{-4}}$	4.3068	SBP- $\Omega[21, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} $	4.6551			
SBP- $\Omega[16, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}}$	3.7176	SBP- $\Omega[21, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} 4$	4.6456			
SBP- $\Omega[16, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}}9$	3.4044	SBP- $\Omega[24, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} $	4.6054			
SBP- Γ [21, 3, 5, 3]_ $\mathcal{E}_{D_{\xi}, 2}$ _2	4.5966	SBP- $\Omega[24, 4, 9, 4]_{\mathcal{E}_{D_{\xi}, 2}}$	4.7272			
SBP- Γ [24, 3, 7, 3]_ $\mathcal{E}_{D_{\xi}, 2}$ _3	2.8462	SBP- $\Omega[24, 4, 9, 4]_{\mathcal{E}_{D_{\xi}, 2}}9$	3.5819			
SBP-diag(E)[20, 3, 5, 3]_ $\mathcal{E}_{D_{\xi}, 2}$ _1	4.0759	SBP- $\Omega[24, 4, 9, 4]_{\mathcal{E}_{D_{\xi}, 2}}10$	5.2262			
SBP-diag(E)[24, 3, 7, 3]_ $\mathcal{E}_{D_{\xi}, 2}_{2}$	3.6320	SBP- $\Gamma[36, 4, 9, 4]_{\mathcal{E}_{D_{\xi}, 2}}5$	4.1362			
-	-	SBP-diag(E)[28,4,7,4]_ $\mathcal{E}_{D_{\xi},2}$ _1	4.9955			
-	-	SBP-diag(E)[36,4,9,4]_ $\mathcal{E}_{D_{\xi},2}_{2}$	4.24855			
_	-	SBP-diag(E)[36, 4, 9, 4]_ $\mathcal{E}_{D_{\mathcal{E}}, 2}$ _3	3.9885			

Table 9Experimental rates of convergence of the SBP operators tested for the Gaussianpulse problem on the periodic curvilinear grid.

3. Efficiency Results

For the p = 1 case, the SBP- Γ and SBP-diag(E) operators have significantly lower error than the LG and LGL nodes due to greater degrees of freedom admitted by their larger number of nodes, which improves their relative efficiency. Also, the efficiency of the SAT computations for these operators aids their efficiency compared to the LG operator. For the p = 2 case, the SBP- $\Omega[8,2,5,2]_{\mathcal{E}_{D_{\xi},2}}$ operator asymptotes to the same efficiency curve as the LG p = 2 operator; this is likely due to their similar error properties and quantity of volume nodes. The SBP- Γ and SBP-diag(E) operators show improved efficiency over the LGL p = 2 operator, again this is likely due to their efficient SAT computations and their lower relative solution error compared to the LGL operator. For the p = 3 case, the SBP- $\Omega[13,3,7,3]_{\mathcal{E}_{D_{\xi},2}}$ operator offers the best computational efficiency, which can be attributed to its low solution error and the few number of nodes in the node set. For the p = 4 case, the LG p = 4 and SBP- $\Omega[24,4,9,4]_{\mathcal{E}_{D_{\xi},2}}$ operators offer the best computational efficiency on quadrilateral elements for this specific degree.



Fig. 5 Solution error for the linear advection equation with an initial Gaussian pulse for degrees p = 1, 2, 3 and 4.



Fig. 6 Efficiency for the linear advection equation with an initial Gaussian pulse for degrees p = 1, 2, 3 and 4.

B. Two-Dimensional Compressible Euler Equations: Isentropic Vortex

1. Problem Definition

For the nonlinear case, we consider the advection of an isentropic vortex as shown in [33]. The compressible Euler equations in two dimensions are given as

$$\frac{\partial \rho}{\partial t} + \sum_{j=1}^{2} \frac{\partial \rho \mathbf{u}_{j}}{\partial x_{j}} = 0$$

$$\frac{\partial \rho \mathbf{u}_{i}}{\partial t} + \sum_{j=1}^{2} \frac{\partial (\rho \mathbf{u}_{i} \mathbf{u}_{j} + p \delta_{ij})}{\partial x_{j}} = 0, \quad i = 1, \dots, 2$$

$$\frac{\partial E}{\partial t} + \sum_{j=1}^{2} \frac{\partial (\mathbf{u}_{j}(E+p))}{\partial x_{j}} = 0,$$
(23)

where ρ is density, $\mathbf{u} = (\mathbf{u}_1, \mathbf{u}_2)$ is the vector of velocities, and *E* is the total energy per unit mass. The pressure *p* is given by the equation of state

$$p = (\gamma - 1) \left(E - \frac{1}{2} \rho \sum_{j=1}^{2} \mathbf{u}_{j}^{2} \right).$$

The analytical solution of the isentropic vortex is given as

$$\rho(\mathbf{x},t) = \left(1 - \frac{\frac{1}{2}(\gamma - 1)(\beta e^{1 - r(\mathbf{x},t)^2})^2}{8\gamma \pi^2}\right)^{\frac{1}{\gamma - 1}}, \quad p = \rho^{\gamma}$$
$$u(\mathbf{x},t) = 1 - \frac{\beta}{2\pi} e^{1 - r(\mathbf{x},t)^2} (y - y_0), \quad v(\mathbf{x},t) = \frac{\beta}{2\pi} e^{1 - r(\mathbf{x},t)^2} (x - x_0 - t)$$

where *u* and *v* are the *x* and *y* velocities, and $r(\mathbf{x}, t) = \sqrt{(x - x_0 - t)^2 + (y - y_0)^2}$. For this case, we follow [33] and take $x_0 = 5, y_0 = 5$ and $\beta = 5$. Furthermore, we consider a periodic domain defined on $\Omega \in [0\ 20] \times [-5\ 5]$ and the time domain $t \in [0\ 5]$. Fig. 7 contains the coarsest grid used in this numerical simulation. The curvilinear transformation used in [33] is used and is given as

$$x = \xi + \alpha \cos\left(\frac{\pi}{20}(\xi - 10)\right) \cos\left(\frac{3\pi}{10}\eta\right),$$
$$y = \eta + \alpha \sin\left(\frac{\pi}{5}(x - 10)\right) \cos\left(\frac{\pi}{10}\eta\right),$$

where $\alpha = 1/8$. After discretizing the spatial derivatives with SBP operators, the semi-discrete system is integrated in time using 4th-order Runge-Kutta time integration with a constant CFL of 0.01. Additionally, we utilize upwind numerical fluxes in the computation of the SAT coupling terms.

For the convergence results, five grid levels were constructed resulting in a total of [2500 10000 22500 40000 62500] elements on each level. At each grid level, the norm of the solution error and the CPU time in seconds was recorded, as presented in the following sections.

2. Solution Error Results

The solution error results for the nonlinear case are shown in Fig. 8 and follow a similar trend to the linear case, with the SBP- Ω family generally performing the best except in the p = 1 case. The SBP- Ω [13,3,7,3]_ $\mathcal{E}_{D_{\xi},2}$ _4 and the SBP- Ω [24,4,9,4]_ $\mathcal{E}_{D_{\xi},2}$ _8 operators show improved accuracy over the LG p = 3 and p = 4 operators, while also using 3 and 1 nodes less than the p = 3 and p = 4 LG nodal distributions, respectively. The design order for the tested operators was generally achieved for each order and each operator and the experimental rates of convergence for each of the tested operators is contained in Table 10.



Fig. 7 The coarsest curvilinear grid level used on the domain $[0\ 20] \times [-5\ 5]$ with 50×50 total elements.

Table 10	Experimental	rates of	convergence	of the SI	BP operators	tested for	r the	isen-
tropic vorte	ex problem on	the perio	dic curviline	ar grid.				

<i>p</i> = 1		<i>p</i> = 2	
Name	Rate	Name	Rate
LG p = 1	2.5822	LG p = 2	3.1311
LGL $p = 1$	1.8265	LGL $p = 2$	2.8243
SBP- $\Omega[4, 1, 3, 1]_{\mathcal{E}_{D_{\xi}, 2}}$	2.5822	SBP- $\Omega[8, 2, 5, 2]_{\mathcal{E}_{D_{\xi}, 2}}$	3.1002
SBP- $\Omega[4, 1, 3, 1]_{\mathcal{E}_{D_{\xi}, 2}}^{2}$	2.5743	SBP- $\Omega[9, 2, 5, 2] = \mathcal{E}_{D_{\xi}, 2} = 2$	3.0832
SBP-Γ[12, 1, 3, 1]_ <i>E</i> _{D_ξ,2_} 3	2.1625	SBP- $\Omega[9, 2, 5, 2]_{\mathcal{E}_{D_{\xi}, 2}}$	3.1367
SBP-diag(E)[8, 1, 1, 1]_ $\mathcal{E}_{D_{\xi}, 2}$ _1	1.8516	_	-
SBP-diag(E)[9, 1, 3, 1]_ $\mathcal{E}_{D_{\xi}, 2}_{2}$	2.2392	_	-
<i>p</i> = 3		<i>p</i> = 4	
Name	Rate	Name	Rate
LG $p = 3$	4.1861	LG p = 4	5.3035
LGL $p = 3$	3.9344	LGL $p = 4$	4.7852
SBP- $\Omega[12, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}}1$	4.1417	SBP- $\Omega[20, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} $	5.2564
SBP- $\Omega[12, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}}^{2}$	4.1294	SBP- $\Omega[20, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} \$	5.3123
SBP- $\Omega[13, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}_{4}}$	4.1866	SBP- $\Omega[21, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} $	5.3650
SBP- $\Omega[16, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}_{Z}}4$	4.1871	SBP- $\Omega[21, 4, 9, 4]_{\mathcal{E}_{D_{\xi}, 2}_{4}}$	5.3522
SBP- $\Omega[13, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}}5$	4.4603	SBP- $\Omega[21, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} $	5.1797
SBP- $\Omega[16, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}}$	3.8505	SBP- $\Omega[24, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} \ 7$	4.9404
SBP- $\Omega[16, 3, 7, 3]_{\mathcal{E}_{D_{\xi}, 2}}9$	3.7758	SBP- $\Omega[24, 4, 9, 4] \mathcal{E}_{D_{\xi}, 2} 10$	5.0162
SBP- Γ [24, 3, 7, 3]_ $\mathcal{E}_{D_{\xi}, 2}$ _3	4.1719	SBP- $\Omega[24, 4, 9, 4]_{\mathcal{E}_{D_{\xi}, 2}}$	5.2061
SBP-diag(E)[20, 3, 5, 3]_ $\mathcal{E}_{D_{\xi}, 2}$ _1	3.8439	SBP- $\Omega[24, 4, 9, 4] \& \mathcal{E}_{D_{\xi}, 2} 9$	5.0849
_	_	SBP-Γ[29,4,7,4]_ <i>E</i> _{Dξ,2} _3	5.6376
_	_	SBP-diag(E)[28,4,7,4]_ $\mathcal{E}_{D_{\xi},2}$ _1	4.7752
_		SBP-diag(E)[36,4,9,4]_ $\mathcal{E}_{D_{\xi},2}_2$	5.2472



Fig. 8 Solution error for the isentropic vortex problem for the compressible Euler equations for degrees p = 1, 2, 3 and 4.



Fig. 9 Efficiency for the isentropic vortex problem for the compressible Euler equations for degrees p = 1, 2, 3 and 4.

3. Efficiency Results

The efficiency results for this test case are contained in Fig. 9. We find that the SBP- Ω operators derived generally perform the most efficiently relative to the other operators tested in this study. In particular, the p = 3 and p = 4 cases show clear improvements in efficiency. The SBP- Γ and SBP-diag(E) operators show some efficiency advantage over the tensor-product LGL operators. In general, the efficiency of the operators for this particular test problem follow similar trends to the efficiency of the operators tested for the Gaussian pulse initial condition for the linear advection equation.

XI. Conclusions

We have derived novel non-tensor-product cubature rules for quadrilateral elements which are amenable to constructing three basic families of multidimensional SBP operators: SBP- Ω , SBP- Γ , and SBP-diag(E). The cubature rules were constructed using a nonlinear least-squares optimization procedure, and the cubature rule with the smallest norm of the cubature truncation error term was selected for each symmetry orbit decomposition. Using these point sets, SBP operators for each of the above families was symbolically constructed with free parameters in the matrix operators S_{ξ} and R_j . The free parameters were optimized using a nonlinear optimization procedure which minimized the norm of the first two leading derivative truncation error terms. The result of this procedure was the construction of SBP operators with generally lower norms of the derivative and cubature truncation error coefficients compared to traditional tensor-product nodal distributions employed for SBP operators on quadrilateral elements. This indicates possible preferential accuracy properties that may be exploited to produce a more efficient operator. However, the complete coupling of the element degrees of freedom poses a potential obstacle to improving computational cost.

These novel operators were compared to SBP operators constructed on traditional LG and LGL tensor-product nodal distributions for the linear advection and compressible Euler equations on two-dimensional uniform and curvilinear meshes. The two test cases considered were an initial Gaussian pulse and the isentropic vortex problem, respectively. The solution error and efficiency for each of the operators was presented and compared.

The construction of the novel cubature rules and the results of the experimental tests performed with the optimized non-tensor-product SBP operators produce the following conclusions:

- Non-tensor-product cubature rules can be constructed with fewer nodes and smaller norms of the cubature truncation error coefficients compared to tensor-product cubature rules on quadrilateral elements.
- Multdimensional SBP operators constructed on the non-tensor-product nodes and optimized for minimizing the norm of the first two derivative truncation error coefficients showed a smaller norm of the first two derivative truncation error coefficients than SBP operators constructed on tensor-product LG and LGL nodes.
- 3) Design order was obtained for a majority of the new non-tensor-product SBP operators.
- The SBP-Ω operators generally have equal or better accuracy than the LG and LGL tensor-product SBP operators while using fewer nodes for equal degree operators for both test cases on uniform and curvilinear grids.
- 5) For all degrees, the SBP-Γ and SBP-diag(E) operators have preferential efficiency properties compared to LGL tensor-product operators for both test cases; this may have potential benefits in entropy-stable schemes.
- 6) The optimized non-tensor-product operators had spectral radii of 1 to 2 orders larger than the tensor-product operators which indicates they have a more restrictive time step.

Many of the new operators have spectral radii an order of magnitude or more greater than the tensor-product and non-tensor-product operators which completed the tests. The large spectral radii imposed a time step that was too restrictive and therefore computationally costly; therefore, these cases were not presented in the numerical results. Future work will consider a composite objective function which includes weighted linear combinations of both the norm of the derivative truncation error terms and the spectral radius of derivative operator; or some variation of the latter objective such as the Frobenius norm.

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Nodal Distributions of Numerically Optimized Cubature Rules

Following are the numerically optimized cubature nodal distributions for each SBP family and SBP operator degrees. The volume nodes are indicated with \circ and the facet cubature points are indicated with \blacksquare . Only the operators derived on nodal distributions which resulted in successful solutions are shown here.





p = 2 SBP- Ω non-tensor-product nodal distibutions.



p = 4 SBP- Ω non-tensor-product nodal distibutions.

SBP-Γ



p = 1 SBP- Γ non-tensor-product nodal distibutions.



p = 2 SBP- Γ non-tensor-product nodal distibutions.



p = 3 SBP- Γ non-tensor-product nodal distibutions.



p = 4 SBP- Γ non-tensor-product nodal distibutions.



p = 1 SBP-diag(E)non-tensor-product nodal distibutions.



SBP-diag(E)[**16,2,5,2**]_ $\mathcal{E}_{D_{\xi},2}$ _**1**

p = 2 SBP-diag(E) non-tensor-product nodal distibutions.



p = 3 SBP-diag(E) non-tensor-product nodal distibutions.



p = 4 SBP-diag(E) non-tensor-product nodal distibutions.

References

- Kreiss, H.-O., and Oliger, J., "Comparison of accurate methods for the integration of hyperbolic equations," *Tellus*, Vol. 24, No. 3, 1972, pp. 199–215.
- [2] Swartz, B., and Wendroff, B., "The relative efficiency of finite difference and finite element methods. I: Hyperbolic problems and splines," *SIAM Journal on Numerical Analysis*, Vol. 11, No. 5, 1974, pp. 979–993.
- [3] Wang, Z. J., Fidkowski, K., Abgrall, R., Bassi, F., Caraeni, D., Cary, A., Deconinck, H., Hartmann, R., Hillewaert, K., Huynh, H. T., and Kroll, N., "High-order CFD methods: current status and perspective," *International Journal for Numerical Methods* in Fluids, Vol. 72, No. 8, 2013, pp. 811–845.
- [4] Kreiss, H.-O., and Scherer, G., "Finite Element and Finite Difference Methods for Hyperbolic Partial Differential Equations," *Mathematical Aspects of Finite Elements in Partal Differential Equations*, Academic Press, New York/London, 1974, pp. 195–212.
- [5] Strand, B., "Summation by Parts for Finite Difference Approximations for d/dx," *Journal of Scientific Computing*, Vol. 20, No. 1, 1994, pp. 47–67.
- [6] Funaro, D., and Gottlieb, D., "A New Method of Imposing Boundary Conditions in Pseudospectral Approximations of Hyperbolic Conservation Laws," *Mathematics of Computation*, Vol. 51, No. 184, 1988, pp. 599–613.
- [7] Carpenter, M. H., Gottlieb, D., and Abarbanel, S., "Time-Stable Boundary Conditions for Finite-Difference Schemes Solving Hyperbolic Systems: Methodology and Application to High-Order Compact Schemes," *Journal of Computational Physics*, Vol. 111, No. 2, 1994, pp. 220–236.
- [8] Osusky, M., and Zingg, D. W., "Parallel Newton-Krylov-Schur Solver for the Navier-Stokes Equations Discretized Using Summation-By-Parts Operators," AIAA Journal, Vol. 51, No. 12, 2013, pp. 2833–2851.
- [9] Diener, P., Dorband, E. N., Schnetter, E., and Tiglio, M., "Optimized High-Order Derivative and Dissipation Operators Satisfying Summation by Parts, and Applications in Three-dimensional Multi-block Evolutions," *Journal of Scientific Computing*, Vol. 32, No. 1, 2007, pp. 109–145.
- [10] Carpenter, M. H., and Gottlieb, D., "Spectral Methods on Arbitrary Grids," *Journal of Computational Physics*, Vol. 129, No. 1, 1996, pp. 74–86.
- [11] Gassner, G. J., "A Skew-Symmetric Discontinuous Galerkin Spectral Element Discretization and Its Relation to SBP-SAT Finite Difference Methods," *SIAM Journal on Scientific Computing*, Vol. 35, No. 3, 2013, pp. A1233–A1253.
- [12] Svärd, M., and Nordström, J., "Finite volume methods, unstructured meshes and strict stability for hyperbolic problems," *Applied Numerical Mathematics*, Vol. 45, 2003, pp. 453–473.
- [13] Ranocha, H., Öffner, P., and Sonar, T., "Summation-by-parts operators for correction procedure via reconstruction," *Journal of Computational Physics*, Vol. 311, 2015, pp. 299–328.
- [14] Del Rey Fernández, D. C., Boom, P. D., and Zingg, D. W., "A generalized framework for nodal first derivative summation-by-parts operators," *Journal of Computational Physics*, Vol. 266, 2014, pp. 214–239.
- [15] Del Rey Fernández, D. C., and Zingg, D. W., "Generalized Summation-by-Parts Operators for the Second Derivative," SIAM Journal on Scientific Computing, Vol. 37, No. 6, 2015, pp. A1840–A1864.
- [16] Hicken, J. E., and Zingg, D. W., "Summation-by-parts operators and high-order quadrature," *Journal of Computational and Applied Mathematics*, Vol. 237, No. 1, 2013, pp. 111–125.
- [17] Hicken, J. E., Del Rey Fernández, D. C., and Zingg, D. W., "Multidimensional Summation-by-Parts Operators: General Theory and Application to Simplex Elements," *SIAM Journal on Scientific Computing*, Vol. 38, No. 4, 2016, pp. A1935–A1958.
- [18] Del Rey Fernández, D. C., Hicken, J. E., and Zingg, D. W., "Simultaneous Approximation Terms for Multi-dimensional Summation-by-Parts Operators," *Journal of Scientific Computing*, Vol. 75, 2018, pp. 83–110.
- [19] Albin, N., and Klarmann, J., "An Algorithmic Exploration of the Existence of High-Order Summation by Parts Operators with Diagonal Norm," *Journal of Scientific Computing*, Vol. 69, 2016, pp. 633–650.
- [20] Mattsson, K., Almquist, M., and Carpenter, M. H., "Optimal diagonal-norm SBP operators," *Journal of Computational Physics*, Vol. 264, 2014, pp. 91–111.

- [21] Mattsson, K., Almquist, M., and van der Weide, E., "Boundary optimized diagonal-norm SBP operators," *Journal of Computational Physics*, Vol. 374, 2018, pp. 1261–1266.
- [22] Cools, R., "Monomial cubature rules since "Stroud": a compilation," *Journal of Computational and Applied Mathematics*, Vol. 48, 1993, pp. 309–326.
- [23] Dunavant, D. A., "Economical Symmetrical Quadrature Rules for Complete Polynomials Over a Square Domain," *International Journal for Numerical Methods in Engineering*, Vol. 21, 1985, pp. 1777–1784.
- [24] Dunavant, D. A., "Efficient Symmetrical Cubature Rules for Complete Polynomials of High Degree Over the Unit Cube," *International Journal for Numerical Methods in Engineering*, Vol. 23, 1986, pp. 397–407.
- [25] Kopriva, D. A., and Gassner, G., "On the Quadrature and Weak Form Choices in Collocation Type Discontinuous Galerkin Spectral Element Methods," *Journal of Scientific Computing*, Vol. 44, 2010, pp. 136–155.
- [26] Kopriva, D. A., and Gassner, G., "A Comparison of the Dispersion and Dissipation Errors of Gauss and Gauss-Lobatto Discontinuous Galerkin Spectral Element Methods," *Journal of Scientific Computing*, Vol. 44, 2010, pp. 136–155.
- [27] Witherden, F. D., and Vincent, P. E., "On the identification of symmetric quadrature rules for finite element methods," *Computers and Mathematics with Applications*, Vol. 69, 2015, pp. 1232–1241.
- [28] Di Pietro, D. A., and Ern, A. (eds.), Mathematical Aspects of Discontinuous Galerkin Methods, Mathematics and Applications, Springer, Heidelberg/Dordrecht/London/New York, 2010, pp. 7, 9.
- [29] Chen, T., and Shu, C.-W., "Entropy stable high order discontinuous Galerkin maethods with suitable quadrature rules for hyperbolic laws," *Journal of Computational Physics*, Vol. 345, 2017, pp. 427–461.
- [30] Del Rey Fernández, D. C., Boom, P. D., Shademan, M., and Zingg, D. W., "Numerical Investigation of Tensor-Product Summation-by-Parts Discretization Strategies and Operators," 55th AIAA Aerospace Sciences Meeting, 2017-0530, 2017.
- [31] Friedrich, L., Del Rey Fernández, D. C., Winters, A. R., Gassner, G., Zingg, D. W., and Hicken, J. E., "Conservative and Stable Degree Preserving SBP Operators for Non-conforming Meshes," *Journal of Scientific Computing*, Vol. 75, 2018, pp. 657–686.
- [32] Friedrich, L., Winters, A. R., Del Rey Fernández, D. C., Gassner, G., Parsani, M., and Carpenter, M. H., "An Entropy Stable h/p Non-Conforming Discontinuous Galerkin Method with the Summation-by-Parts Property," *SIAM Journal on Scientific Computing*, Vol. 345, 2017, pp. 1–37.
- [33] Chan, J., Del Rey Fernández, D. C., and Carpenter, M. H., "Efficient entropy stable Gauss collocation methods," *arXiv:1809.01178*, 2018.
- [34] Carpenter, M. H., Fisher, T. C., Nielsen, E. J., and Frankel, S. H., "Entropy Stable Spectral Collocation Schemes for the Navier-Stokes Equations: Discontinuous Interfaces," Tech. Rep. NF1676L-17321, NASA, 2014.
- [35] Zhang, L., Cui, T., and Liu, H., "A Set of Symmetric Quadrature Rules on Triangles and Tetrahedra," *Journal of Computational Mathematics*, Vol. 27, 2009, pp. 89–96.