

1 EFFICIENT ENTROPY STABLE GAUSS COLLOCATION METHODS

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3 **Abstract.** The construction of high order entropy stable collocation schemes on quadrilateral
4 and hexahedral elements has relied on the use of Gauss-Legendre-Lobatto collocation points [1, 2, 3]
5 and their equivalence with summation-by-parts (SBP) finite difference operators [4]. In this work,
6 we show how to efficiently generalize the construction of semi-discretely entropy stable schemes on
7 tensor product elements to Gauss points and generalized SBP operators. Numerical experiments
8 suggest that the use of Gauss points can significantly improve accuracy on curved meshes.

9 **1. Introduction.** Time dependent nonlinear conservation laws are ubiquitous in
10 computational fluid dynamics (CFD), for which high order methods are increasingly of
11 interest. Such methods are more accurate per degree of freedom than low order meth-
12 ods, while also possessing much smaller numerical dispersion and dissipation errors.
13 This makes high order methods especially well suited to time-dependent simulations.
14 In this work, we focus specifically on discontinuous Galerkin methods on unstruc-
15 tured quadrilateral and hexahedral meshes. These methods combine properties of
16 high order approximations with the geometric flexibility of unstructured meshing.

17 However, high order methods are notorious for being more prone to instability
18 compared to low order methods [5]. This instability is addressed through various
19 stabilization techniques (e.g. artificial viscosity, filtering, slope limiting). However,
20 these techniques often reduce accuracy to first or second order, and can prevent solvers
21 from realizing the advantages of high order approximations. Moreover, it is often not
22 possible to prove that a high order scheme does not blow up even in the presence of
23 stabilization. This ambiguity can necessitate the re-tuning of stabilization parameters,
24 as parameters which are both stable and accurate for one problem or discretization
25 setting may provide either too little or too much numerical dissipation for another.

26 The instability of high order methods is rooted in the fact that discretizations of
27 nonlinear conservation laws do not typically satisfy a discrete analogue of the conser-
28 vation or dissipation of energy (entropy). While the numerical dissipation present for
29 low order methods serves as a stabilizing mechanism, the low of numerical dissipation
30 in high order methods reveals the lack of an inherent statement of stability. The
31 dissipation of entropy serves as an energetic principle for nonlinear conservation laws
32 [6], and requires the use of the chain rule in its proof. The instability of high order
33 methods is tied to the fact that, when discretizing systems of nonlinear PDEs, the
34 chain rule does not typically hold at the discrete level.

35 The lack of a chain rule was circumvented by using a non-standard “flux differenc-
36 ing” formulation [1, 2, 3, 7], which is key to constructing semi-discretely entropy stable
37 high order schemes on unstructured quadrilateral and hexahedral meshes. Flux dif-
38 ferencing replaces the derivative of the nonlinear flux with the discrete differentiation
39 of an auxiliary quantity. This auxiliary quantity is computed through the evaluation
40 of a two-point entropy conservative flux [8] using pairs of solution values at quadra-
41 ture points. These entropy stable schemes were later extended to non-tensor product
42 elements using GLL-like quadrature points on triangles and tetrahedra [9, 10]. More
43 recently, the construction of efficient entropy stable schemes was extended to more
44 arbitrary choices of basis and quadrature [11, 12].

45 This paper focuses on the construction of efficient semi-discretely entropy stable
46 collocation schemes based on Gauss nodes, using the framework introduced in [11, 12].
47 While entropy stable collocation schemes have been constructed on Gauss-like quadra-

ture points without boundary nodes [13], the inter-element coupling terms for such schemes introduce significantly more communication and computation than collocation points which contain boundary nodes. This work introduces new inter-element coupling terms which avoid this all-to-all coupling, requiring only communication of face values between neighboring elements.

In Section 2, we briefly review the derivation of continuous entropy inequalities for systems of nonlinear conservation laws. In Section 3, we describe how to construct entropy stable discretizations of nonlinear conservation laws using different quadrature points on affine tensor product elements. In Section 4, we describe how to extend this construction to curvilinear elements, and Section 5 presents numerical results which confirm the high order accuracy and stability of the proposed method for smooth, discontinuous, and under-resolved (turbulent) solutions of the compressible Euler equations in two and three dimensions.

2. A brief review of entropy stability theory. We are interested in methods for the numerical solution of systems of conservation laws in d dimensions

$$(2.1) \quad \frac{\partial \mathbf{u}}{\partial t} + \sum_{i=1}^d \frac{\partial \mathbf{f}_i(\mathbf{u})}{\partial x_i} = 0,$$

where \mathbf{u} denotes the conservative variables, $\mathbf{f}_i(\mathbf{u})$ are nonlinear fluxes, and x_i denotes the i th coordinate. Many physically motivated conservation laws admit a statement of stability involving a convex scalar entropy $S(\mathbf{u})$. We first define the entropy variables $\mathbf{v}(\mathbf{u})$ to be the gradient of the entropy $S(\mathbf{u})$ with respect to the conservative variables

$$\mathbf{v} = \frac{\partial S(\mathbf{u})}{\partial \mathbf{u}}.$$

For a convex entropy, $\mathbf{v}(\mathbf{u})$ defines an invertible mapping from conservative to entropy variables. We denote the inverse of this mapping (from entropy to conservative variables) by $\mathbf{u}(\mathbf{v})$.

At the continuous level, it can be shown (for example, in [6]) that vanishing viscosity solutions to (2.1) satisfy the strong form of an entropy inequality

$$(2.2) \quad \frac{\partial S(\mathbf{u})}{\partial t} + \sum_{i=1}^d \frac{\partial F_i(\mathbf{u})}{\partial x_i} \leq 0,$$

where F_i denotes the i th scalar entropy flux function and $\psi_i(\mathbf{u})$ denotes the i th entropy potential

$$F_i(\mathbf{u}) = \mathbf{v}^T \frac{\partial \mathbf{f}_i}{\partial x_i}, \quad \psi_i(\mathbf{u}) = \mathbf{v}^T \mathbf{f}_i(\mathbf{u}) - F_i(\mathbf{u}).$$

Integrating (2.2) over a domain Ω and applying the divergence theorem yields an integrated entropy inequality

$$(2.3) \quad \int_{\Omega} \frac{\partial S(\mathbf{u})}{\partial t} + \int_{\partial \Omega} \sum_{i=1}^d \mathbf{n}_i (\mathbf{v}^T \mathbf{f}_i(\mathbf{u}) - \psi_i(\mathbf{u})) \leq 0,$$

where $\partial \Omega$ denotes the boundary of Ω and \mathbf{n}_i denotes the i th component of the outward normal on $\partial \Omega$. Roughly speaking, this implies that the time rate of change of entropy is less than or equal to the flux of entropy through the boundary.

3. Entropy stable Gauss and Gauss-Legendre-Lobatto collocation methods. This focus of this paper is on entropy stable high order collocation methods which satisfy a semi-discrete version of the entropy inequality (2.3). These methods collocate the solution at some choice of collocation nodes, and are applicable to tensor product meshes consisting of quadrilateral and hexahedral elements.

Entropy stable collocation methods have largely utilized Gauss-Legendre-Lobatto (GLL) nodes [1, 2, 3, 7], which contain points on the boundary. The popularity of GLL nodes can be attributed in part to a connection made in [4], where it was shown by Gassner that collocation DG discretizations based on GLL nodes could be recast in terms of summation-by-parts (SBP) operators. This equivalence allowed Gassner to leverage existing finite difference formulations to produce stable high order discretizations of the nonlinear Burgers' equation.

GLL quadratures contain boundary points, which greatly simplifies the construction of inter-element coupling terms for entropy stable collocation schemes. However, it is also known that the use of GLL quadrature within DG methods under-integrates the mass matrix, which can lead to solution “aliasing” and lower accuracy [14]. In this work, we explore entropy stable collocation schemes based on Gauss quadrature points instead of GLL points.

This comparison is motivated by the accuracy of each respective quadrature rule. While $(N + 1)$ -point GLL quadrature rules are exact for polynomial integrands of degree $(2N - 1)$, $(N + 1)$ -point Gauss quadrature rules are exact for polynomials of degree $(2N + 1)$. This higher accuracy of Gauss quadrature has been shown to translate to lower errors and slightly improved rates of convergence in simulations of wave propagation and fluid flow [15, 16, 17]. However, Gauss points have not been widely used to construct entropy stable discretizations due to the lack of efficient, stable, and high order accurate inter-element coupling terms, known as simultaneous approximation terms (SBP-SAT) in the finite difference literature [18, 13, 19]. SBP-SATs for Gauss points are non-compact, in the sense that they introduce all-to-all coupling between degrees of freedom on neighboring elements. This results in greater communication between elements, as well as a significantly larger number of two-point flux evaluations and floating point operations.

It is possible to realize the improved accuracy of Gauss points while avoiding non-compact SBP-SATs through a staggered grid formulation, where the solution is stored at Gauss nodes but interpolated to a set of higher degree $(N + 2)$ GLL “flux” points for computation [14]. Because GLL nodes include boundary points, compact and high order accurate SBP-SAT terms can be constructed for the flux points. After performing computations on the flux points, the results are interpolated back to Gauss points and used to evolve the solution forward in time. Figure 1 shows an illustration of GLL, staggered grid, and Gauss point sets for a 2D quadrilateral element.

The following sections will describe how to construct efficient high order entropy stable schemes using Gauss points. These schemes are based on “decoupled” SBP operators introduced in [11, 12], which are applicable to general choices of basis and quadrature. By choosing a tensor product Lagrange polynomial basis and $(N + 1)$ point Gauss quadrature rules, we recover a Gauss collocation scheme. The high order accuracy and entropy stability of this scheme are direct results of theorems presented in [11, 12]. However, we will also present a different proof of entropy stability in one dimension for completeness.

3.1. Gauss nodes and generalized summation by parts operators. We assume the solution is collocated at $(N + 1)$ quadrature points x_i with associated

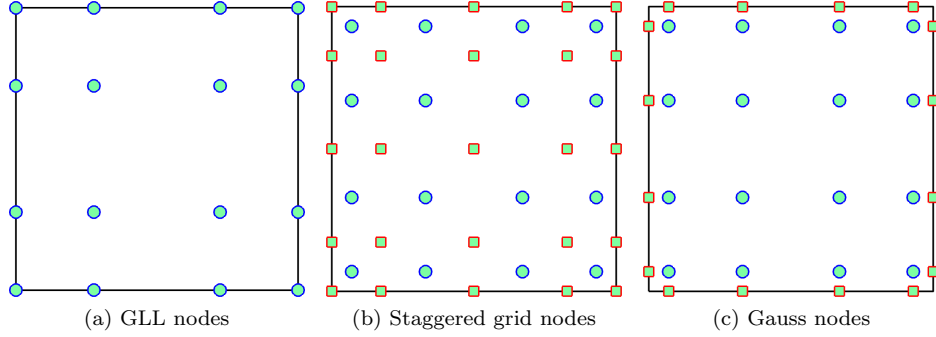


Fig. 1: Examples of nodal sets under which efficient entropy stable schemes can be constructed. This work focuses on the construction of efficient and accurate SBP-SAT terms for Gauss nodal sets.

quadrature weights w_i . We do not make any assumptions on the points, in order to accommodate both GLL and Gauss nodes using this notation. The collocation assumption is equivalent to approximating the solution using a degree N Lagrange basis $\ell_j(x)$ defined over the $(N + 1)$ quadrature points.

Let \mathbf{D} denote the nodal differentiation matrix, and let \mathbf{V}_f denote the $(N + 1) \times 2$ matrix which interpolates polynomials at Gauss nodes to values at endpoints. These two matrices are defined entrywise as

$$D_{ij} = \left. \frac{\partial \ell_j}{\partial x} \right|_{x=x_i}, \quad (\mathbf{V}_f)_{i1} = \ell_i(-1), \quad (\mathbf{V}_f)_{i2} = \ell_i(1).$$

We also introduce the diagonal matrix of quadrature weights $\mathbf{W}_{ij} = \delta_{ij} w_i$. In this work, \mathbf{W} is identical to the mass matrix, whose entries are evaluated as L^2 inner products of basis functions. This equality holds so long as the basis functions are Lagrange polynomials and integrals are approximated using quadrature (either GLL or Gauss). It can be shown that the mass and differentiation matrices for Gauss nodes fall under the class of generalized SBP (GSBP) operators [20].

LEMMA 3.1. $\mathbf{Q} = \mathbf{W}\mathbf{D}$ satisfies the generalized summation by parts property

$$\mathbf{Q} = \mathbf{V}_f^T \mathbf{B} \mathbf{V}_f - \mathbf{Q}^T, \quad \mathbf{B} = \begin{bmatrix} -1 & \\ & 1 \end{bmatrix}.$$

The proof is a direct restatement of integration by parts, and can be found in [21, 22, 23]. Lemma 3.1 holds for both GLL and Gauss nodes, and switching between these two nodal sets simply results in a redefinition of the matrices \mathbf{D}, \mathbf{V}_f . For example, because GLL nodes include boundary points, the interpolation matrix \mathbf{V}_f reduces to a generalized permutation matrix which extracts the nodal values associated with the left and right endpoints.

3.2. Existing entropy stable SBP-SATs for generalized SBP operators.

In this section, we will review the construction of semi-discretely entropy stable discretizations. Entropy stable discretizations can be constructed by first introducing an entropy conservative scheme, then adding appropriate interface dissipation to produce

an entropy inequality. The construction of entropy conservative schemes relies on the existence of an two-point (dyadic) entropy conservative flux [8].

DEFINITION 3.2. Let $\mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R)$ be a bivariate function which is symmetric and consistent with the flux function $\mathbf{f}(\mathbf{u})$

$$\mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R) = \mathbf{f}_S(\mathbf{u}_R, \mathbf{u}_L), \quad \mathbf{f}_S(\mathbf{u}, \mathbf{u}) = \mathbf{f}(\mathbf{u})$$

The numerical flux $\mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R)$ is entropy conservative if, for entropy variables $\mathbf{v}_L = \mathbf{v}(\mathbf{u}_L)$, $\mathbf{v}_R = \mathbf{v}(\mathbf{u}_R)$, the Tadmor “shuffle” condition is satisfied

$$(\mathbf{v}_L - \mathbf{v}_R)^T \mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R) = (\psi_L - \psi_R), \quad \psi_L = \psi(\mathbf{v}(\mathbf{u}_L)), \quad \psi_R = \psi(\mathbf{v}(\mathbf{u}_R)).$$

For illustrative purposes, we will prove a semi-discrete entropy inequality on a one-dimensional mesh consisting of two elements of degree N . We assume both meshes are translations of a reference element $[-1, 1]$, such that derivatives with respect to physical coordinates are identical to derivatives with respect to reference coordinates. The extension to multiple elements and variable mesh sizes is straightforward.

The construction of entropy conservative schemes relies on appropriate SBP-SATs for Gauss collocation schemes [18, 13, 19]. Let the rows of \mathbf{V}_f be denoted as $\mathbf{t}_L, \mathbf{t}_R$

$$\mathbf{V}_f = \begin{bmatrix} - & \mathbf{t}_L & - \\ - & \mathbf{t}_R & - \end{bmatrix}, \quad (\mathbf{t}_L)_j = \ell_j(-1), \quad (\mathbf{t}_R)_j = \ell_j(1).$$

The inter-element coupling terms in [18, 13, 19] utilize a decomposition of the surface mass matrix $\mathbf{V}_f^T \mathbf{B} \mathbf{V}_f$ as

$$(3.1) \quad \mathbf{V}_f^T \mathbf{B} \mathbf{V}_f = \mathbf{t}_R \mathbf{t}_R^T - \mathbf{t}_L \mathbf{t}_L^T.$$

The construction of entropy conservative schemes on multiple elements requires appropriate inter-element coupling terms (SBP-SATs) involving $\mathbf{t}_L, \mathbf{t}_R$. We consider a two element mesh, and show how SBP-SATs can be interpreted as constructing a global SBP operator.

Let $\mathbf{u}_N^1, \mathbf{u}_N^2$ denote nodal degrees of freedom of the vector valued solution $\mathbf{u}(x)$ on the first and second element, respectively. To simplify notation, we assume that all following operators are defined in terms of Kronecker products, such that they are applied to each component of $\mathbf{u}_N^1, \mathbf{u}_N^2$. We first define the matrix

$$(3.2) \quad \mathbf{S} = \mathbf{Q} - \frac{1}{2} \mathbf{V}_f^T \mathbf{B} \mathbf{V}_f.$$

It is straightforward to show (using Lemma 3.1) that \mathbf{S} is skew-symmetric. We can now define an SBP operator $\mathbf{D}_h = \mathbf{W}_h^{-1} \mathbf{Q}_h$ over two elements

$$(3.3) \quad \mathbf{Q}_h = \underbrace{\begin{bmatrix} \mathbf{S} & \frac{1}{2} \mathbf{t}_R \mathbf{t}_L^T \\ -\frac{1}{2} \mathbf{t}_L \mathbf{t}_R^T & \mathbf{S} \end{bmatrix}}_{\mathbf{S}_h} + \underbrace{\begin{bmatrix} -\frac{1}{2} \mathbf{t}_L \mathbf{t}_L^T & \\ & \frac{1}{2} \mathbf{t}_R \mathbf{t}_R^T \end{bmatrix}}_{\frac{1}{2} \mathbf{B}_h}, \quad \mathbf{W}_h = \begin{bmatrix} \mathbf{W} & \\ & \mathbf{W} \end{bmatrix}.$$

It can be shown that \mathbf{D}_h is high order accurate such that, if \mathbf{u}_h is a polynomial of degree N , it is differentiated exactly. Straightforward computations show that \mathbf{Q}_h also satisfies an SBP property $\mathbf{Q}_h + \mathbf{Q}_h^T = \mathbf{B}_h$.

196 Ignoring boundary conditions, an entropy conservative scheme for (2.1) on two
 197 elements can then be given as

$$198 \quad (3.4) \quad \frac{d}{dt} \mathbf{W}_h \mathbf{u}_h + 2(\mathbf{Q}_h \circ \mathbf{F}_S) \mathbf{1} = 0, \quad \mathbf{u}_h = \begin{bmatrix} \mathbf{u}_N^1 \\ \mathbf{u}_N^2 \end{bmatrix}$$

$$199 \quad (\mathbf{F}_S)_{ij} = \mathbf{f}_S((\mathbf{u}_h)_i, (\mathbf{u}_h)_j), \quad 1 \leq i, j \leq 2(N+1).$$

201 where \circ denotes the Hadamard product [24]. Multiplying (3.4) by $\mathbf{v}_h^T = \mathbf{v}(\mathbf{u}_h)^T$ will
 202 yield a semi-discrete version of the conservation of entropy (mimicking (2.3) with the
 203 inequality replaced by an equality)

$$204 \quad (3.5) \quad \frac{d}{dt} \mathbf{W}_h S(\mathbf{u}_h) + \mathbf{v}_h^T (\mathbf{B}_h \circ \mathbf{F}_S) \mathbf{1} - \mathbf{1}^T \mathbf{B}_h \psi(\mathbf{u}_h) = 0.$$

205 We refer to [13, 10] for the proof of (3.5).

206 The drawback of the SBP-SATs introduced in this section lies in the nature
 207 of the off-diagonal matrices $\mathbf{t}_R \mathbf{t}_L$ and $-\mathbf{t}_L \mathbf{t}_R$. For Gauss nodes, these blocks are
 208 dense, which implies that inter-element coupling terms produce a non-compact stencil.
 209 Evaluating (3.4) requires computing two-point fluxes \mathbf{f}_S between all nodes on two
 210 neighboring elements, which significantly increases both the computational work, as
 211 well as communication between neighboring elements. The main goal of this work is
 212 to circumvent the all-to-all coupling of degrees of freedom introduced by the SBP-
 213 SATs described in this section, which can be done through the use of “decoupled”
 214 SBP operators.

215 **3.3. Decoupled SBP operators.** Decoupled SBP operators were first intro-
 216 duced in [11] and used to construct entropy stable schemes on simplicial elements.
 217 These operators (and simplifications under a collocation assumption) are presented
 218 in a more general setting in [11, 12] and in Appendix A. In this section, decoupled
 219 SBP operators are introduced in one dimension for GLL and Gauss nodal sets.

220 Decoupled SBP operators build upon the GSBP matrices \mathbf{W}, \mathbf{Q} , interpolation
 221 matrix \mathbf{V}_f , and boundary matrix \mathbf{B} introduced in Section 3.1. The decoupled SBP
 222 operator \mathbf{Q}_N is defined as the block matrix

$$223 \quad (3.6) \quad \mathbf{Q}_N = \begin{bmatrix} \mathbf{Q} - \frac{1}{2} \mathbf{V}_f^T \mathbf{B} \mathbf{V}_f & \frac{1}{2} \mathbf{V}_f^T \mathbf{B} \\ -\frac{1}{2} \mathbf{B} \mathbf{V}_f & \frac{1}{2} \mathbf{B} \end{bmatrix}.$$

224 Lemma 3.1 and straightforward computations show that \mathbf{Q}_N also satisfies the follow-
 225 ing SBP property

226 LEMMA 3.3. Let \mathbf{Q}_N be defined through (3.6). Then,

$$227 \quad \mathbf{Q}_N + \mathbf{Q}_N^T = \begin{bmatrix} \mathbf{0} & \\ & \mathbf{B} \end{bmatrix}.$$

228 The matrix \mathbf{Q}_N acts not only on volume nodes, but on both volume and surface
 229 nodes. However, \mathbf{Q}_N does not directly define an approximation to the derivative. Let
 230 $f(x), g(x)$ denote two functions, and let \mathbf{f}, \mathbf{g} denote the values of f, g at interior nodal
 231 points. We also define vectors $\mathbf{f}_N, \mathbf{g}_N$ denoting the values of f, g at both interior and

232 boundary points

$$233 \quad (3.7) \quad \mathbf{f}_N = \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_{N+1}) \\ f(-1) \\ f(1) \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{f}_f \end{bmatrix}, \quad \mathbf{g}_N = \begin{bmatrix} g(x_1) \\ \vdots \\ g(x_{N+1}) \\ g(-1) \\ g(1) \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ \mathbf{g}_f \end{bmatrix}.$$

234 Then, a polynomial approximation to $f \frac{\partial g}{\partial x}$ can be computed using \mathbf{Q}_N . Let \mathbf{u} denote
 235 the nodal values of the polynomial $u(x) \approx f \frac{\partial g}{\partial x}$. These coefficients are computed via

$$236 \quad (3.8) \quad \mathbf{W}\mathbf{u} = \begin{bmatrix} \mathbf{I} \\ \mathbf{V}_f \end{bmatrix}^T \text{diag}(\mathbf{f}_N) \mathbf{Q}_N \mathbf{g}_N.$$

237 The expression (3.8) can be rewritten in “strong” form as follows

$$\begin{aligned} 238 \quad \mathbf{u} &= \mathbf{W}^{-1} \begin{bmatrix} \mathbf{I} \\ \mathbf{V}_f \end{bmatrix}^T \text{diag}(\mathbf{f}_N) \mathbf{Q}_N \mathbf{g}_N \\ 239 \quad &= \text{diag}(\mathbf{f}) \mathbf{D} \mathbf{g} + \frac{1}{2} \text{diag}(\mathbf{f}) \mathbf{W}^{-1} \mathbf{V}_f^T \mathbf{B} (\mathbf{g}_f - \mathbf{V}_f \mathbf{g}) \\ 240 \quad &\quad + \frac{1}{2} \mathbf{W}^{-1} \mathbf{V}_f^T \mathbf{B} \text{diag}(\mathbf{f}_f) (\mathbf{g}_f - \mathbf{V}_f \mathbf{g}), \end{aligned}$$

242 where we have used the fact that diagonal matrices commute to simplify expressions.
 243 The decoupled SBP operator \mathbf{Q}_N can thus be interpreted as adding boundary correc-
 244 tions to the GSBP operator \mathbf{D} in a skew-symmetric fashion.

245 It was shown in [11] that \mathbf{u} is a high order accurate approximation to the quantity
 246 $f \frac{\partial g}{\partial x}$. Both the generalized SBP operator \mathbf{D} and the expression in (3.8) involving the
 247 decoupled SBP operator recover exact derivatives of high order polynomials. However,
 248 when applied to non-polynomial functions, the decoupled SBP operator \mathbf{Q}_N improves
 249 accuracy near the boundaries. Figure 2 illustrates this by using both operators to
 250 approximate the derivative of a Gaussian e^{-4x^2} . The decoupled SBP operator results
 251 in an improved approximation near the boundary.

252 **3.4. An entropy stable Gauss collocation scheme based on decoupled**
 253 **SBP operators.** We can now construct an entropy conservative Gauss collocation
 254 scheme with compact SBP-SATs using decoupled SBP operators. As in Section 3.2,
 255 we will construct a Gauss collocation scheme and provide a proof of semi-discrete
 256 entropy conservation for a two-element mesh.

257 (see Figure ??) [Add pics of two-element mesh](#)

258 We first note that \mathbf{B} can be trivially decomposed into the sum of two outer
 259 products as in (3.1)

$$260 \quad (3.9) \quad \mathbf{B} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} = \mathbf{e}_R \mathbf{e}_R^T - \mathbf{e}_L \mathbf{e}_L^T, \quad \mathbf{e}_L = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \mathbf{e}_R = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

261 The vectors $\mathbf{e}_L, \mathbf{e}_R$ are related to $\mathbf{t}_L, \mathbf{t}_R$ through the interpolation matrix \mathbf{V}_f . Because
 262 $\mathbf{t}_L, \mathbf{t}_R$ are rows of \mathbf{V}_f , $\mathbf{t}_L \mathbf{1} = \mathbf{t}_R \mathbf{1} = 1$. This can be used to show, for example, that

$$263 \quad (3.10) \quad \mathbf{B} \mathbf{V}_f \mathbf{1} = (\mathbf{e}_R \mathbf{e}_R^T - \mathbf{e}_L \mathbf{e}_L^T) \mathbf{1} = \mathbf{e}_R - \mathbf{e}_L.$$

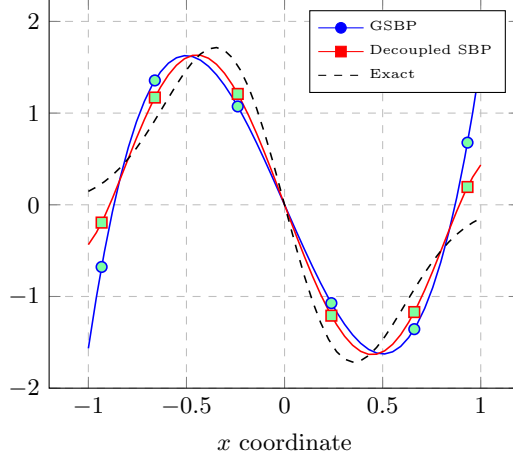


Fig. 2: Degree $N = 5$ approximations of derivatives of a Gaussian e^{-4x^2} using the generalized SBP operator \mathbf{D} and the decoupled SBP operator \mathbf{Q}_N via (3.8). The colored circles and squares denote values at Gauss points.

We can define a decoupled SBP matrix \mathbf{Q}_h over two elements as follows

$$(3.11) \quad \mathbf{Q}_h = \left[\begin{array}{cc|cc} \mathbf{S} & \frac{1}{2}\mathbf{V}_f^T\mathbf{B} & & \\ -\frac{1}{2}\mathbf{B}\mathbf{V}_f & -\frac{1}{2}\mathbf{e}_L\mathbf{e}_L^T & \frac{1}{2}\mathbf{e}_R\mathbf{e}_L^T & \\ \hline & -\frac{1}{2}\mathbf{e}_L\mathbf{e}_R^T & \mathbf{S} & \frac{1}{2}\mathbf{V}_f^T\mathbf{B} \\ & & -\frac{1}{2}\mathbf{B}\mathbf{V}_f & \frac{1}{2}\mathbf{e}_R\mathbf{e}_R^T \end{array} \right]$$

We can also show that $\mathbf{Q}_h\mathbf{1} = 0$. Using (3.10), we have that

$$(3.12) \quad \mathbf{Q}_h\mathbf{1} = \left[\begin{array}{c} (\mathbf{S} + \frac{1}{2}\mathbf{V}_f^T\mathbf{B})\mathbf{1} \\ \frac{1}{2}\mathbf{B}\mathbf{V}_f\mathbf{1} + \frac{1}{2}(\mathbf{e}_R - \mathbf{e}_L) \\ (\mathbf{S} + \frac{1}{2}\mathbf{V}_f^T\mathbf{B})\mathbf{1} \\ \frac{1}{2}\mathbf{B}\mathbf{V}_f\mathbf{1} + \frac{1}{2}(\mathbf{e}_R - \mathbf{e}_L) \end{array} \right] = \left[\begin{array}{c} (\mathbf{Q} - \frac{1}{2}\mathbf{V}_f^T\mathbf{B}\mathbf{V}_f + \frac{1}{2}\mathbf{V}_f^T\mathbf{B}\mathbf{V}_f)\mathbf{1} \\ \frac{1}{2}\mathbf{B}(-\mathbf{1} + \mathbf{1}) \\ (\mathbf{Q} - \frac{1}{2}\mathbf{V}_f^T\mathbf{B}\mathbf{V}_f + \frac{1}{2}\mathbf{V}_f^T\mathbf{B}\mathbf{V}_f)\mathbf{1} \\ \frac{1}{2}\mathbf{B}(-\mathbf{1} + \mathbf{1}) \end{array} \right] = \mathbf{0}.$$

Here, we have used the definition of \mathbf{B} in (3.9), the fact that $\mathbf{V}_f\mathbf{1} = \mathbf{1}$ and $\mathbf{Q}\mathbf{1} = 0$ [20], and the definition of \mathbf{S} in (3.2). This property (3.12) will be used in the proof of entropy conservation.

It can be helpful to split up \mathbf{Q}_h into two matrices

$$(3.13) \quad \mathbf{Q}_h = \mathbf{S}_h + \frac{1}{2}\mathbf{B}_h, \quad \mathbf{S}_h = \left[\begin{array}{cc|cc} \mathbf{S} & \frac{1}{2}\mathbf{V}_f^T\mathbf{B} & & \\ -\frac{1}{2}\mathbf{B}\mathbf{V}_f & -\frac{1}{2}\mathbf{e}_L\mathbf{e}_L^T & \frac{1}{2}\mathbf{e}_R\mathbf{e}_L^T & \\ \hline & -\frac{1}{2}\mathbf{e}_L\mathbf{e}_R^T & \mathbf{S} & \frac{1}{2}\mathbf{V}_f^T\mathbf{B} \\ & & -\frac{1}{2}\mathbf{B}\mathbf{V}_f & \frac{1}{2}\mathbf{e}_R\mathbf{e}_R^T \end{array} \right]$$

$$\mathbf{B}_h = \left[\begin{array}{c|c} -\mathbf{e}_L\mathbf{e}_L^T & \\ \hline & \mathbf{e}_R\mathbf{e}_R^T \end{array} \right].$$

The matrix \mathbf{S}_h is skew-symmetric, while the matrix \mathbf{B}_h functions as a boundary operator which extracts boundary values over the two-element domain (i.e. \mathbf{B}_h extracts

a left boundary value from element 1 and a right boundary value from element 2).
 Note that here, \mathbf{B}_h is diagonal, unlike the boundary operator defined in Section 3.2.
 The two-element decoupled SBP operator \mathbf{Q}_h in (3.11) is related to the GSBP operator in (3.3) through a block interpolation matrix

$$\mathbf{I}_h = \begin{bmatrix} \mathbf{I} & \\ \mathbf{V}_f & \mathbf{I} \\ & \mathbf{V}_f \end{bmatrix}, \quad \mathbf{I}_h^T \mathbf{Q}_h \mathbf{I}_h = \begin{bmatrix} \mathbf{S} & \frac{1}{2} \mathbf{t}_R \mathbf{t}_L^T \\ -\frac{1}{2} \mathbf{t}_L \mathbf{t}_R^T & \mathbf{S} \end{bmatrix} + \begin{bmatrix} -\frac{1}{2} \mathbf{t}_L \mathbf{t}_L^T & \\ & \frac{1}{2} \mathbf{t}_R \mathbf{t}_R^T \end{bmatrix}.$$

Let $\mathbf{u}_N^1, \mathbf{u}_N^2$ denote the values of the conservative variables at Gauss points on elements 1 and 2, respectively, and let \mathbf{u}_h denote their concatenation as defined in (3.4). Let $\mathbf{v}(\mathbf{u}_N^i)$ denote the evaluation of entropy variables at Gauss points on element i , and define the “entropy-projected conservative variables” $\tilde{\mathbf{u}}_f^1, \tilde{\mathbf{u}}_f^2$ by evaluating the conservative variables in terms of the interpolated values of the entropy variables at element boundaries

$$\tilde{\mathbf{u}}_f^i = \mathbf{u}(\mathbf{v}_f^i), \quad \mathbf{v}_f^i = \mathbf{V}_f \mathbf{v}(\mathbf{u}_N^i), \quad i = 1, 2.$$

We now introduce $\mathbf{u}_h = [\mathbf{u}_N^1 \quad \mathbf{u}_N^2]^T$ as the concatenated vector of solution values at Gauss points, and define $\mathbf{v}_h, \tilde{\mathbf{v}}$, and $\tilde{\mathbf{u}}$ as follows:

$$\mathbf{v}_h = \mathbf{v}(\mathbf{u}_h) = \mathbf{v} \left(\begin{bmatrix} \mathbf{u}_N^1 \\ \mathbf{u}_N^2 \end{bmatrix} \right), \quad \tilde{\mathbf{v}} = \mathbf{I}_h \mathbf{v}_h, \quad \tilde{\mathbf{u}} = \mathbf{u}(\tilde{\mathbf{v}}) = \begin{bmatrix} \mathbf{u}_N^1 \\ \tilde{\mathbf{u}}_f^1 \\ \mathbf{u}_N^2 \\ \tilde{\mathbf{u}}_f^2 \end{bmatrix}.$$

The term \mathbf{v}_h corresponds to the vector of entropy variables at \mathbf{u}_h , while $\tilde{\mathbf{v}}$ corresponds to the concatenated vector of Gauss point values and interpolated boundary values \mathbf{v}_f^i of the entropy variables. The term $\tilde{\mathbf{u}}$ denotes the evaluation of the conservative variables in terms of $\tilde{\mathbf{v}}$.

Finally, we define \mathbf{F}_S as the matrix of evaluations of the two-point flux \mathbf{f}_S at combinations of values of $\tilde{\mathbf{u}}$

$$(\mathbf{F}_S)_{ij} = \mathbf{f}_S(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_j), \quad 1 \leq i, j \leq 2(N+3).$$

Note that, due to the consistency of \mathbf{f}_S , the diagonal of \mathbf{F}_S reduces to flux evaluations

$$(3.13) \quad (\mathbf{F}_S)_{ii} = \mathbf{f}_S(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_i) = \mathbf{f}(\tilde{\mathbf{u}}_i).$$

We can now construct a semi-discretely entropy conservative formulation based on decoupled SBP operators:

THEOREM 3.4. *Let \mathbf{Q}_h be defined by (3.11), and let \mathbf{u}_h denote the two-element solution of the following formulation*

$$(3.14) \quad \mathbf{W}_h \frac{d}{dt} \mathbf{u}_h + \mathbf{I}_h^T (\mathbf{Q}_h \circ \mathbf{F}_S) \mathbf{1} = 0.$$

Then, \mathbf{u}_h satisfies a semi-discrete conservation of entropy

$$\mathbf{1}^T \mathbf{W}_h \frac{dS(\mathbf{u}_h)}{dt} + \mathbf{1}^T \mathbf{B}_h (\mathbf{v}_f^T \mathbf{f}(\tilde{\mathbf{u}}_f) - \psi(\tilde{\mathbf{u}}_f)) = 0$$

$$\mathbf{v}_f = \begin{bmatrix} \mathbf{t}_L \mathbf{v}(\mathbf{u}_N^1) \\ \mathbf{t}_R \mathbf{v}(\mathbf{u}_N^2) \end{bmatrix}, \quad \tilde{\mathbf{u}}_f = \mathbf{u}(\mathbf{v}_f).$$

313 *Proof.* The proof results from testing with \mathbf{v}_h^T . Since $\mathbf{v}(\mathbf{u}) = \frac{\partial S(\mathbf{u})}{\partial \mathbf{u}}$ and \mathbf{W}_h is
 314 diagonal, the time term yields

$$315 \quad \mathbf{v}_h^T \frac{d}{dt} \mathbf{W}_h \mathbf{u}_h = \mathbf{1}^T \frac{d}{dt} \mathbf{W}_h \text{diag}(\mathbf{v}_h) \mathbf{u}_h = \mathbf{1}^T \frac{d}{dt} \mathbf{W}_h S(\mathbf{u}_h).$$

316 The spatial term can be manipulated as follows

$$317 \quad 2\mathbf{v}_h^T \mathbf{I}_h^T (\mathbf{Q}_h \circ \mathbf{F}_S) \mathbf{1} = 2(\mathbf{I}_h \mathbf{v}_h)^T \left((\mathbf{S}_h \circ \mathbf{F}_S) \mathbf{1} + \frac{1}{2} (\mathbf{B}_h \circ \mathbf{F}_S) \mathbf{1} \right) \\
 318 \quad = \tilde{\mathbf{v}}^T (\mathbf{B}_h \circ \mathbf{F}_S) \mathbf{1} + \tilde{\mathbf{v}}^T (\mathbf{S}_h \circ \mathbf{F}_S) \mathbf{1} - \mathbf{1}^T (\mathbf{S}_h \circ \mathbf{F}_S) \tilde{\mathbf{v}},$$

320 where we have used the skew-symmetry of \mathbf{S}_h in the last step. The boundary term
 321 reduces to

$$322 \quad \tilde{\mathbf{v}}^T (\mathbf{B}_h \circ \mathbf{F}_S) \mathbf{1} = \mathbf{1}^T \mathbf{B}_h \tilde{\mathbf{v}}_f^T \mathbf{f}(\tilde{\mathbf{u}}),$$

323 where we have used (3.13) and the fact that \mathbf{B}_h is diagonal. Here, $\tilde{\mathbf{v}}_f^T \mathbf{f}(\tilde{\mathbf{u}})$ denotes a
 324 vector whose entries are the inner product of $\tilde{\mathbf{v}}$ and $\mathbf{f}(\tilde{\mathbf{u}})$ at face points.

325 The volume terms can be manipulated using the definition of \mathbf{F}_S and the Tadmor
 326 shuffle condition in Definition 3.2

$$327 \quad \tilde{\mathbf{v}}^T (\mathbf{S}_h \circ \mathbf{F}_S) \mathbf{1} - \mathbf{1}^T (\mathbf{S}_h \circ \mathbf{F}_S) \tilde{\mathbf{v}} = \sum_{ij} (\mathbf{S}_h)_{ij} (\tilde{\mathbf{v}}_i - \tilde{\mathbf{v}}_j)^T \mathbf{f}_S(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_j) \\
 328 \quad = \sum_{ij} (\mathbf{S}_h)_{ij} (\psi(\tilde{\mathbf{u}}_i) - \psi(\tilde{\mathbf{u}}_j)) \\
 329 \quad = \psi(\tilde{\mathbf{u}})^T \mathbf{S}_h \mathbf{1} - \mathbf{1}^T \mathbf{S}_h \psi(\tilde{\mathbf{u}}) = 2 \left(\psi(\tilde{\mathbf{u}})^T \mathbf{S}_h \mathbf{1} \right).$$

331 where we have again used the skew-symmetry of \mathbf{S}_h in the last step. Substituting
 332 $\mathbf{S}_h = \mathbf{Q}_h - \frac{1}{2} \mathbf{B}_h$ and using (3.12) yields

$$333 \quad 2 \left(\psi(\tilde{\mathbf{u}})^T \mathbf{S}_h \mathbf{1} \right) = \psi(\tilde{\mathbf{u}})^T (2\mathbf{Q}_h - \mathbf{B}_h) \mathbf{1} = -\psi(\tilde{\mathbf{u}})^T \mathbf{B}_h \mathbf{1} = -\mathbf{1}^T \mathbf{B}_h \psi(\tilde{\mathbf{u}}),$$

334 where we have used the symmetry of \mathbf{B}_h in the last step. \square

335 **REMARK.** The proof of Theorem 3.4 follows directly from choosing either GLL
 336 or Gauss quadratures in Theorem 4 of [11]. The proof is reproduced here for clarity,
 337 as the two-element case illuminates the skew-symmetric nature and structure of the
 338 inter-element coupling more explicitly.

339 It is possible to convert the semi-discrete entropy equality in Theorem 3.4 to a
 340 semi-discrete entropy inequality by adding appropriate interface dissipation terms,
 341 such as Lax-Friedrichs or matrix dissipation [25]. We note that these terms must be
 342 computed in terms of $\tilde{\mathbf{u}}_f$ in order to ensure a discrete dissipation of entropy [9, 11].

343 **4. Extension to higher dimensions and curved meshes.** The formulation
 344 in Theorem 3.4 can be naturally extended to Cartesian meshes in higher dimensions
 345 through a tensor product construction. We consider first the construction of higher
 346 dimensional differentiation matrices on a two-dimensional reference element \hat{D} , as-
 347 suming a two dimensional tensor product grid of quadrature nodes (the construction
 348 of decoupled SBP operators in three dimensions is straightforward and similar to the
 349 two-dimensional case). We then construct physical differentiation matrices on mapped
 350 elements D^k , through which we construct an entropy conservative scheme.

Let $\mathbf{D}_{1D}, \mathbf{W}_{1D}$ denote the 1D differentiation and mass matrices, respectively, on the reference interval $[-1, 1]$. Let \mathbf{W} denote the 2D reference mass matrix, and let \mathbf{D}^i denote the differentiation matrices with respect to the i th reference coordinate. These matrices can be expressed in terms of Kronecker products

$$\mathbf{D}^1 = \mathbf{D}_{1D} \otimes \mathbf{I}_{N+1}, \quad \mathbf{D}^2 = \mathbf{I}_{N+1} \otimes \mathbf{D}_{1D}, \quad \mathbf{W} = \mathbf{W}_{1D} \otimes \mathbf{W}_{1D}.$$

where \mathbf{I}_{N+1} denotes the $(N+1) \times (N+1)$ identity matrix.

We also construct higher dimensional face interpolation matrices. Let $\mathbf{V}_{f,1D}$ denote the one-dimensional interpolation matrix, and let \mathbf{B}_{1D} denote the boundary matrix defined in Lemma 3.1. For an appropriate ordering of face quadrature points, the two-dimensional face interpolation matrix \mathbf{V}_f and reference boundary matrices $\mathbf{B}^1, \mathbf{B}^2$ can be expressed as the concatenation of Kronecker product matrices

$$\mathbf{V}_f = \begin{bmatrix} \mathbf{V}_{f,1D} \otimes \mathbf{I}_2 \\ \mathbf{I}_2 \otimes \mathbf{V}_{f,1D} \end{bmatrix}, \quad \mathbf{B}^1 = \begin{bmatrix} \mathbf{B}_{1D} \otimes \mathbf{I}_2 & \\ & \mathbf{0} \end{bmatrix}, \quad \mathbf{B}^2 = \begin{bmatrix} \mathbf{0} & \\ & \mathbf{I}_2 \otimes \mathbf{B}_{1D} \end{bmatrix}.$$

In three dimensions, the face interpolation matrix would be expressed as the concatenation of three Kronecker products involving $\mathbf{V}_{f,1D}$. The higher dimensional differentiation and interpolation matrices $\mathbf{D}^i, \mathbf{V}_f$ can now be used to construct higher dimensional decoupled SBP operators. Let \mathbf{Q}_N^i denote the decoupled SBP operator for the i th coordinate on the reference element, where \mathbf{Q}_N^i is defined as

$$\mathbf{Q}_N^i = \begin{bmatrix} \mathbf{Q}^i - \frac{1}{2} \mathbf{V}_f^T \mathbf{B}^i \mathbf{V}_f & \frac{1}{2} \mathbf{V}_f^T \mathbf{B}^i \\ -\frac{1}{2} \mathbf{B}^i \mathbf{V}_f & \frac{1}{2} \mathbf{B}^i \end{bmatrix}, \quad \mathbf{Q}^i = \mathbf{W} \mathbf{D}^i.$$

Let the domain now be decomposed into non-overlapping elements D^k , such that D^k is the image of \widehat{D} under a degree N polynomial mapping Φ^k . We define geometric terms \mathbf{G}_{ij}^k as scaled derivatives of reference coordinates $\widehat{\mathbf{x}}$ with respect to physical coordinates \mathbf{x}

$$J^k \mathbf{G}_{ij}^k = J^k \frac{\partial \widehat{x}_j}{\partial x_i},$$

where J^k is the determinant of the Jacobian of Φ^k . We also introduce the face Jacobian J_f^k , which is computed from the mapping of a physical face to a reference face. We define matrices over each physical element D^k

$$\mathbf{W}_k = \mathbf{W} \text{diag}(\mathbf{J}^k), \quad \mathbf{B}_k^i = \mathbf{B}_N^i \text{diag}(\mathbf{n}_i \circ \mathbf{J}^f)$$

$$\mathbf{Q}_k^i = \frac{1}{2} \sum_{j=1}^d \left(\text{diag}(\widetilde{\mathbf{G}}_{ij}^k) \mathbf{Q}_N^i + \mathbf{Q}_N^i \text{diag}(\widetilde{\mathbf{G}}_{ij}^k) \right),$$

where we have discretized the differentiation matrix in split form [26]. Here, \mathbf{J}^k denotes the vector of values of J^k at volume quadrature points, $\widetilde{\mathbf{G}}_{ij}^k$ denotes the vector of values of $J^k \mathbf{G}_{ij}^k$ at volume and face quadrature points, and $\mathbf{n}_i^k, \mathbf{J}_f^k$ denote the i th outward unit normal and J_f^k at face quadrature points. Then, an entropy conservative scheme in two dimensions is given as follows:

THEOREM 4.1. Assume that $\mathbf{Q}^k \mathbf{1} = 0$. Let \mathbf{u}_N^k denote the solution on D^k satis-

386 *fying*

$$\begin{aligned}
387 \quad & \sum_k \left(\mathbf{W}_k \frac{d\mathbf{u}_N^k}{dt} + \sum_{i=1}^d \left(2(\mathbf{Q}_k^i \circ \mathbf{F}_S) + \mathbf{V}_f^T \mathbf{B}_k^i \mathbf{f}_S(\tilde{\mathbf{u}}_f^+, \tilde{\mathbf{u}}_f^k) \right) \right) = 0 \\
388 \quad & (\mathbf{F}_S)_{ij} = \mathbf{f}_S(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_j), \quad \tilde{\mathbf{u}} = \begin{bmatrix} \mathbf{u}_N^k \\ \tilde{\mathbf{u}}_f^k \end{bmatrix}, \quad \tilde{\mathbf{u}}_f^k = \mathbf{u}(\mathbf{v}_f^k), \quad \mathbf{v}_f^k = \mathbf{V}_f \mathbf{v}(\mathbf{u}_N^k), \\
389
\end{aligned}$$

390 where $\tilde{\mathbf{u}}^+$ denotes boundary values of the entropy-projected conservative variables on
391 neighboring elements. Then, \mathbf{u}_N^k satisfies the discrete conservation of entropy

$$392 \quad \sum_k \left(\mathbf{1}^T \mathbf{W} \frac{d\mathbf{u}_N^k}{dt} + \sum_{i=1}^d \mathbf{1}^T \mathbf{B}^i (\mathbf{v}_f^T \mathbf{f}(\tilde{\mathbf{u}}_f) - \psi(\tilde{\mathbf{u}}_f)) \right) = 0.$$

393 *Proof.* The proof is a special case of the proof of Theorem 1 in [12]. \square

394 We note that Theorem 4.1 relies on the assumption that $\mathbf{Q}^k \mathbf{1} = 0$. This condition
395 is equivalent to ensuring that the scaled geometric terms $\tilde{\mathbf{G}}_{ij}^k$ satisfy a discrete geo-
396 metric conservation law (GCL) [2, 7, 10, 12]. For two-dimensional degree N (isopara-
397 metric) mappings, the GCL is automatically satisfied. However, in three dimensions,
398 the GCL is not guaranteed to be satisfied at the discrete level, due to the fact that
399 geometric terms for isoparametric mappings are polynomials of degree higher than N .

400 It is possible to ensure the satisfaction of a discrete GCL by using a sub-parametric
401 polynomial geometric mapping. Let N_{geo} denote the degree of a polynomial geometric
402 mapping. In three dimensions, the exact geometric terms for a degree N_{geo} polynomial
403 mapping are polynomials of degree $(2N_{\text{geo}} - 2)$ [27, 16, 10]. If $(2N_{\text{geo}} - 2) \leq N$, or if
404 $N_{\text{geo}} \leq \lfloor \frac{N}{2} \rfloor + 1$, then the discrete GCL is automatically satisfied.

405 For $N_{\text{geo}} \geq \lfloor \frac{N}{2} \rfloor + 1$, modifications to the computation of geometric terms are
406 required to ensure that the GCL is satisfied at the discrete level. For general SBP op-
407 erators, the discrete GCL can be enforced through the solution of a local least squares
408 problem [10]. We take an alternative approach and construct geometric terms using
409 the approach of Kopriva [27]. This construction takes advantage of the fact that GLL
410 and Gauss collocation methods correspond to polynomial discretizations. Kopriva's
411 construction is based on rewriting the geometric terms as the curl of some auxiliary
412 quantity. By approximating this auxiliary quantity using polynomial interpolation
413 prior to applying the curl, the geometric terms are approximated by degree N poly-
414 nomials which satisfy the discrete GCL by construction.

415 To summarize, entropy stable Gauss collocation schemes on curved meshes require
416 the following additional steps:

- 417 1. Construct polynomial approximations of the geometric terms at GLL nodes
418 using (??) [27].
- 419 2. Evaluate the geometric terms at volume and surface quadrature points.
- 420 3. Compute normal vectors using (??).

5. Numerical results. The compressible Euler equations in d dimensions are given as follows:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \sum_{j=1}^d \frac{\partial (\rho \mathbf{u}_j)}{\partial x_j} &= 0, \\ \frac{\partial \rho \mathbf{u}_i}{\partial t} + \sum_{j=1}^d \frac{\partial (\rho \mathbf{u}_i \mathbf{u}_j + p \delta_{ij})}{\partial x_j} &= 0, \quad i = 1, \dots, d \\ \frac{\partial E}{\partial t} + \sum_{j=1}^d \frac{\partial (\mathbf{u}_j (E + p))}{\partial x_j} &= 0. \end{aligned}$$

Here, ρ is density, $\mathbf{u} = (\mathbf{u}_1, \dots, \mathbf{u}_d)$ is the vector of velocities, and E is the total energy. The pressure p and specific internal energy ρe are given by

$$p = (\gamma - 1) \left(E - \frac{1}{2} \rho |\mathbf{u}|^2 \right), \quad \rho e = E - \frac{1}{2} \rho |\mathbf{u}|^2, \quad |\mathbf{u}|^2 = \left(\sum_{j=1}^d \mathbf{u}_j^2 \right).$$

There exists an infinite family of suitable convex entropies for the compressible Euler equations [28]. However, there is only a single unique entropy which appropriately treats the viscous heat conduction term in the compressible Navier-Stokes equations [29]. This entropy $S(\mathbf{u})$ is given in d dimensions by

$$S(\mathbf{u}) = -\frac{\rho s}{\gamma - 1},$$

where $s = \log \left(\frac{p}{\rho^\gamma} \right)$ is the physical specific entropy. The entropy variables in d dimensions are given by

$$\begin{aligned} v_1 &= \frac{\rho e (\gamma + 1 - s) - E}{\rho e}, \\ v_{1+i} &= \frac{\rho \mathbf{u}_i}{\rho e}, \quad i = 1, \dots, d, \\ v_{d+2} &= -\frac{\rho}{\rho e}, \end{aligned}$$

while the conservation variables in terms of the entropy variables are given by

$$\begin{aligned} \rho &= -(\rho e) v_{d+2}, \\ \rho \mathbf{u}_i &= (\rho e) v_{1+i}, \quad i = 1, \dots, d \\ E &= (\rho e) \left(1 - \frac{\sum_{j=1}^d v_{1+j}^2}{2 v_{d+2}} \right), \end{aligned}$$

where the quantities ρe and s in terms of the entropy variables are

$$\rho e = \left(\frac{(\gamma - 1)}{(-v_{d+2})^\gamma} \right)^{1/(\gamma-1)} e^{\frac{-s}{\gamma-1}}, \quad s = \gamma - v_1 + \frac{\sum_{j=1}^d v_{1+j}^2}{2 v_{d+2}}.$$

Explicit expressions for entropy conservative numerical fluxes in two dimensions are

given by Chandrashekar [30]

$$\begin{aligned}
f_{1,S}^1(\mathbf{u}_L, \mathbf{u}_R) &= \{\{\rho\}\}^{\log} \{\{u\}\}, & f_{2,S}^1(\mathbf{u}_L, \mathbf{u}_R) &= \{\{\rho\}\}^{\log} \{\{v\}\}, \\
f_{1,S}^2(\mathbf{u}_L, \mathbf{u}_R) &= f_{1,S}^1 \{\{u\}\} + p_{\text{avg}}, & f_{2,S}^2(\mathbf{u}_L, \mathbf{u}_R) &= f_{2,S}^1 \{\{u\}\}, \\
f_{1,S}^3(\mathbf{u}_L, \mathbf{u}_R) &= f_{2,S}^2, & f_{2,S}^3(\mathbf{u}_L, \mathbf{u}_R) &= f_{2,S}^1 \{\{v\}\} + p_{\text{avg}}, \\
f_{1,S}^4(\mathbf{u}_L, \mathbf{u}_R) &= (E_{\text{avg}} + p_{\text{avg}}) \{\{u\}\}, & f_{2,S}^4(\mathbf{u}_L, \mathbf{u}_R) &= (E_{\text{avg}} + p_{\text{avg}}) \{\{v\}\},
\end{aligned}$$

where we have defined the auxiliary quantities

$$\begin{aligned}
p_{\text{avg}} &= \frac{\{\{\rho\}\}}{2 \{\{\beta\}\}}, & E_{\text{avg}} &= \frac{\{\{\rho\}\}^{\log}}{2 \{\{\beta\}\}^{\log} (\gamma - 1)} + \frac{\|\mathbf{u}\|_{\text{avg}}^2}{2}, \\
\|\mathbf{u}\|_{\text{avg}}^2 &= 2(\{\{u\}\}^2 + \{\{v\}\}^2) - (\{\{u^2\}\} + \{\{v^2\}\}).
\end{aligned}$$

Expressions for entropy conservative numerical fluxes for the three-dimensional compressible Euler equations can also be explicitly written as

$$\begin{aligned}
\mathbf{f}_{1,S} &= \begin{pmatrix} \{\{\rho\}\}^{\log} \{\{u\}\} \\ \{\{\rho\}\}^{\log} \{\{u\}\}^2 + p_{\text{avg}} \\ \{\{\rho\}\}^{\log} \{\{u\}\} \{\{v\}\} \\ \{\{\rho\}\}^{\log} \{\{u\}\} \{\{w\}\} \\ (E_{\text{avg}} + p_{\text{avg}}) \{\{u\}\} \end{pmatrix}, & \mathbf{f}_{2,S} &= \begin{pmatrix} \{\{\rho\}\}^{\log} \{\{v\}\} \\ \{\{\rho\}\}^{\log} \{\{u\}\} \{\{v\}\} \\ \{\{\rho\}\}^{\log} \{\{v\}\}^2 + p_{\text{avg}} \\ \{\{\rho\}\}^{\log} \{\{v\}\} \{\{w\}\} \\ (E_{\text{avg}} + p_{\text{avg}}) \{\{v\}\} \end{pmatrix}, \\
\mathbf{f}_{3,S} &= \begin{pmatrix} \{\{\rho\}\}^{\log} \{\{w\}\} \\ \{\{\rho\}\}^{\log} \{\{u\}\} \{\{w\}\} \\ \{\{\rho\}\}^{\log} \{\{v\}\} \{\{w\}\} \\ \{\{\rho\}\}^{\log} \{\{w\}\}^2 + p_{\text{avg}} \\ (E_{\text{avg}} + p_{\text{avg}}) \{\{w\}\} \end{pmatrix}.
\end{aligned}$$

with auxiliary quantities

$$\begin{aligned}
p_{\text{avg}} &= \frac{\{\{\rho\}\}}{2 \{\{\beta\}\}}, & E_{\text{avg}} &= \frac{\{\{\rho\}\}^{\log}}{2(\gamma - 1) \{\{\beta\}\}^{\log}} + \frac{1}{2} \{\{\rho\}\}^{\log} \|\mathbf{u}\|_{\text{avg}}^2 \\
\|\mathbf{u}\|_{\text{avg}}^2 &= 2(\{\{u\}\}^2 + \{\{v\}\}^2 + \{\{w\}\}^2) - (\{\{u^2\}\} + \{\{v^2\}\} + \{\{w^2\}\}).
\end{aligned}$$

In all problems, we estimate the timestep size dt using J, J^f , and degree-dependent L^2 trace constants C_N

$$dt = C_{\text{CFL}} \frac{h}{C_N}, \quad h = \frac{1}{\|J^{-1}\|_{L^\infty} \|J^f\|_{L^\infty}},$$

where C_{CFL} is some user-defined CFL constant. For isotropic elements, the ratio of J to J^f scales as the mesh size h , while C_N captures the dependence of the maximum stable timestep on the polynomial degree N . For hexahedral elements, C_N varies depending on the choice of quadrature. It was shown in [17] that

$$C_N = \begin{cases} d^{\frac{N(N+1)}{2}} & \text{for GLL nodes} \\ d^{\frac{(N+1)(N+2)}{2}} & \text{for Gauss nodes} \end{cases}.$$

Thus, based on this rough estimate of the maximum stable timestep, GLL collocation schemes should be able to take a timestep which is roughly $(1 + 2/N)$ times larger than

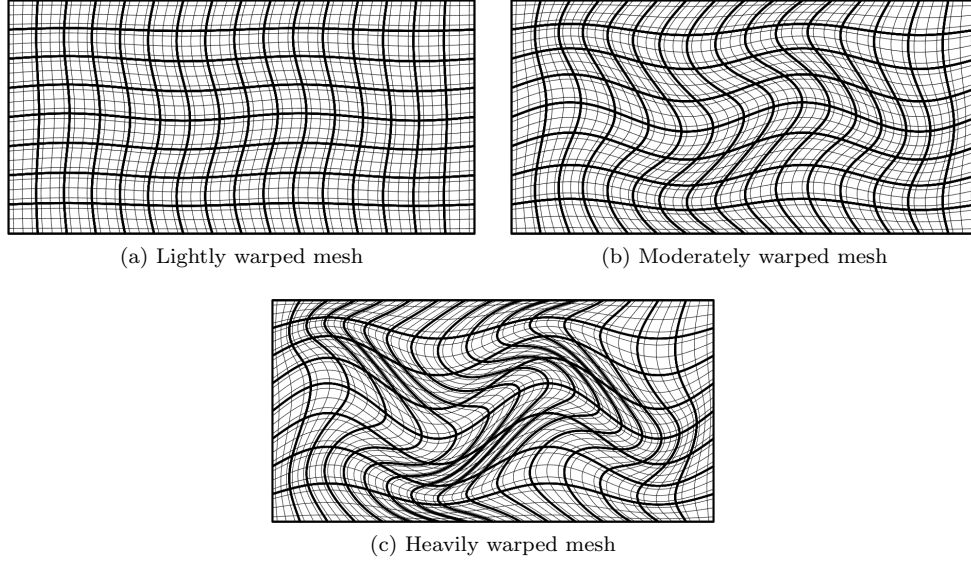


Fig. 3: Lightly, moderately, and heavily warped meshes for $N = 4, K = 16$.

the maximum stable timestep for Gauss collocation schemes. We do not account for this discrepancy in this work, and instead set the timestep for both GLL and Gauss collocation schemes based on the more conservative Gauss collocation estimate of dt .

Numerical results in 1D are similar to those presented in [11]. Thus, we focus on two and three dimensional problems and comparisons of entropy stable GLL and Gauss collocation schemes.

5.1. 2D isentropic vortex problem. We begin by examining high order convergence of the proposed methods in two dimensions using the isentropic vortex problem [31, 13]. The analytical solution is

$$(5.1) \quad \rho(\mathbf{x}, t) = \left(1 - \frac{\frac{1}{2}(\gamma - 1)(\beta e^{1-r(\mathbf{x}, t)^2})^2}{8\gamma\pi^2} \right)^{\frac{1}{\gamma-1}}, \quad p = \rho^\gamma,$$

$$u(\mathbf{x}, t) = 1 - \frac{\beta}{2\pi} e^{1-r(\mathbf{x}, t)^2} (y - y_0), \quad v(\mathbf{x}, t) = \frac{\beta}{2\pi} e^{1-r(\mathbf{x}, t)^2} (y - y_0),$$

where u, v are the x and y velocity and $r(\mathbf{x}, t) = \sqrt{(x - x_0 - t)^2 + (y - y_0)^2}$. Here, we take $x_0 = 5, y_0 = 0$ and $\beta = 5$.

We solve on a periodic rectangular domain $[0, 20] \times [-5, 5]$ until final time $T = 5$, and compute errors over all solution fields. For a degree N approximation, we approximate the L^2 error using an $(N + 2)$ point Gauss quadrature rule. We also examine the influence of element curvature for both GLL and Gauss collocation schemes by examining L^2 errors on a sequence of moderately and heavily warped curvilinear meshes (see Figure 3). These warpings are constructed by modifying

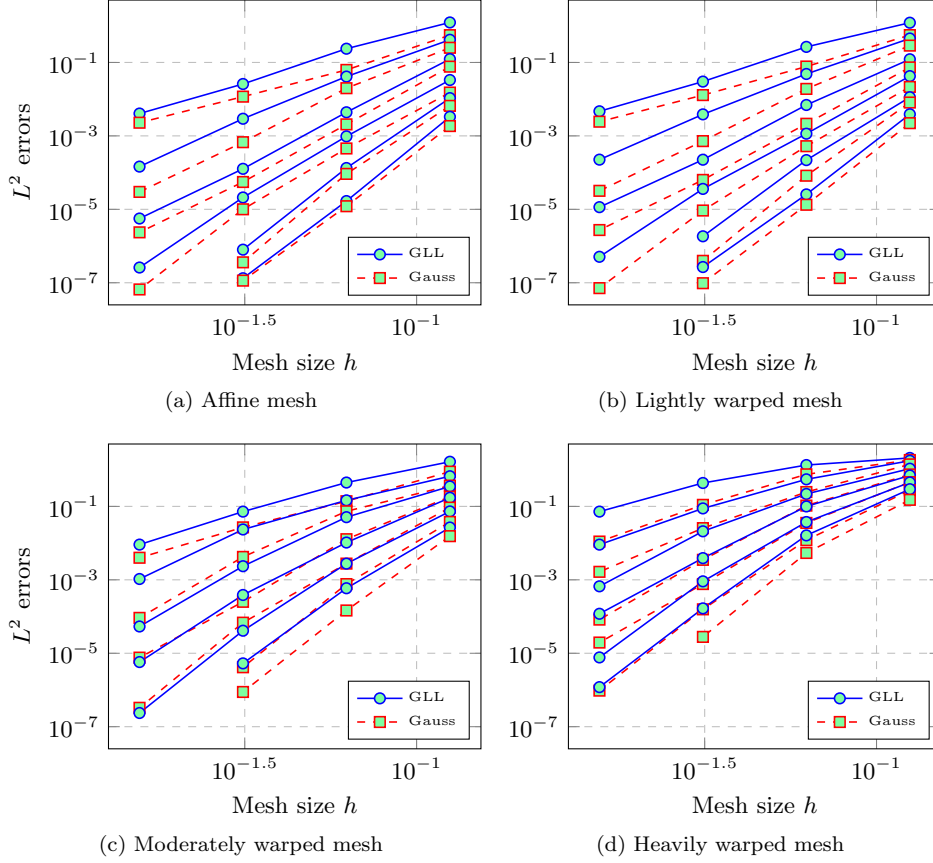


Fig. 4: L^2 errors for the 2D isentropic vortex at time $T = 5$ for degree $N = 2, \dots, 7$ GLL and Gauss collocation schemes.

nodal positions according to the following mapping

$$\begin{aligned}\tilde{x} &= x + \alpha \cos\left(\frac{\pi}{20}(x - 10)\right) \cos\left(\frac{3\pi}{10}y\right) \\ \tilde{y} &= y + \alpha \sin\left(\frac{\pi}{5}(\tilde{x} - 10)\right) \cos\left(\frac{\pi}{10}y\right).\end{aligned}$$

The lightly warped mesh corresponds to $\alpha = 1/32$, the moderately warped mesh corresponds to $\alpha = 1/8$, and the heavily warped mesh corresponds to $\alpha = 1/4$. All results are computed using $C_{\text{CFL}} = 1/2$ and Lax-Friedrichs interface dissipation.

Figure 4 shows the L^2 errors for affine, moderately warped, and heavily warped meshes. For affine meshes, Gauss collocation results in a lower errors than GLL collocation at all orders. However, the difference between both schemes decreases as N increases. This is not too surprising: on a Cartesian domain, the discrete L^2 inner product resulting from GLL quadrature converges to exact L^2 inner product over the space of polynomials as N increases [32]. However, GLL and Gauss collocation differ more significantly on curved meshes. For both moderately and heavily warped meshes, the errors for a degree N Gauss collocation scheme are nearly identical to

errors for a higher order GLL collocation scheme of degree $(N + 1)$. These results are in line with numerical experiments in [14], which show that GLL collocation schemes lose one order of convergence in the L^2 norm on unstructured non-uniform meshes. Both results show that increasing quadrature accuracy significantly reduces the effect of polynomial aliasing due to curved meshes and spatially varying geometric terms.

We note that L^2 approximation estimates on curved meshes [33, 34, 35] assume that the mesh size is small enough to be in the asymptotic regime (such that asymptotic error estimates hold). On curved meshes, this requires that the mesh is sufficiently fine to resolve both the solution and geometric mapping. The numerical results in Figure 4 suggest that, compared to Gauss collocation schemes, under-integrated GLL collocation schemes may require a much finer mesh resolution to reach the asymptotic regime.

5.2. 3D isentropic vortex problem. As in two dimensions, we test the accuracy of the proposed scheme using an isentropic vortex solution adapted to three dimensions. The solution is the extruded 2D vortex propagating in the y direction, with an analytic expression given in [36]

$$\begin{aligned}\rho(\mathbf{x}, t) &= \left(1 - \frac{(\gamma - 1)}{2} \Pi^2\right)^{\frac{1}{\gamma-1}} \\ \mathbf{u}(\mathbf{x}, t) &= \Pi \mathbf{r}, \\ E(\mathbf{x}, t) &= \frac{p_0}{\gamma - 1} \left(1 - \frac{\gamma - 1}{2} \Pi^2\right)^{\frac{\gamma}{\gamma-1}} + \frac{\rho}{2} |\mathbf{u}|.\end{aligned}$$

where $\mathbf{u} = (u, v, w)^T$ is the velocity vector and

$$\Pi = \Pi_{\max} e^{\frac{1-\gamma}{2} \mathbf{r}^T \mathbf{r}}, \quad \mathbf{r} = \begin{pmatrix} -(x_2 - c_2 - t) \\ x_1 - c_1 \\ 0 \end{pmatrix}.$$

We take $c_1 = c_2 = 5$, $p_0 = 1/\gamma$, and $\Pi_{\max} = 0.4$, and solve on the domain $[0, 10] \times [0, 20] \times [0, 10]$. As in the 2D case, we also examine the effect of curvilinear mesh warping. Following [12], we construct a curved warping of the initial Cartesian mesh by mapping nodes on each hexahedron to warped nodal positions $(\tilde{x}, \tilde{y}, \tilde{z})$ through the transformation

$$\tilde{\mathbf{x}} = \mathbf{x} + \sin\left(\pi \frac{(x - 5)}{5}\right) \sin\left(2\pi \frac{(y - 10)}{10}\right) \sin\left(\pi \frac{(z - 5)}{5}\right).$$

On curved meshes, the geometric terms are constructed using the approach of Kopriva described in Section 4. A $C_{\text{CFL}} = .75$ is used for all experiments.

Figure 5 shows the L^2 errors for degrees $N = 2, 3, 4$. As in the 2D case, Gauss collocation schemes produce smaller errors than GLL collocation schemes, especially on curved meshes. The difference between the two schemes on affine meshes is slightly more pronounced than in 2D. The difference between the two schemes on curved meshes is qualitatively similar to the 2D case, with Gauss collocation achieving higher accuracy than GLL collocation schemes at all polynomial degrees and mesh resolutions.

We also compared L^2 errors for both isoparametric and sub-parametric geometric mappings. For sub-parametric mappings, we chose the degree of approximation of geometry $N_{\text{geo}} = \lfloor \frac{N}{2} \rfloor + 1$, such that the geometric terms are computed exactly and

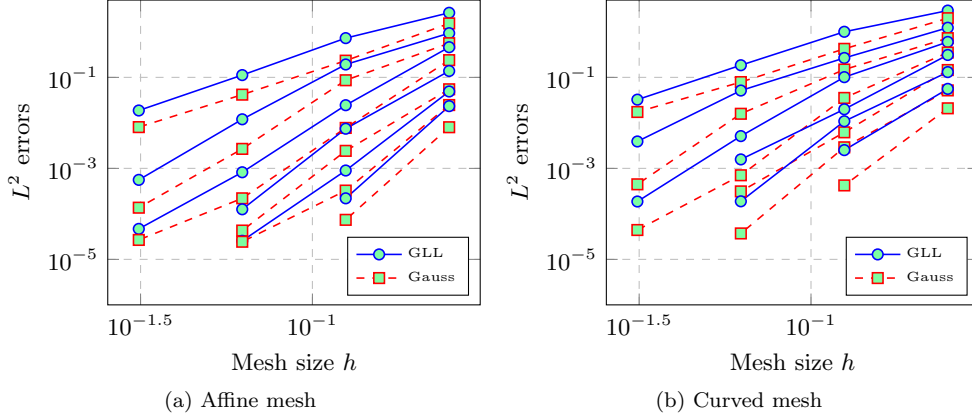


Fig. 5: L^2 errors for the 3D isentropic vortex for $N = 2, \dots, 7$ on sequences of Cartesian and curved meshes.

the GCL is satisfied by default. This test is intended to address the fact that the GCL-preserving interpolation of Kopriva introduces a small approximation error, as the geometric terms are no longer exact. For these sub-parametric mappings, the gap between GLL and Gauss collocation widens slightly at $N = 2$. However, the results for sub-parametric mappings are nearly identical to the results in the isoparametric case for higher polynomial degrees.

5.3. Shock-vortex interaction. describe shock-vortex problem

We modify the shock-vortex interaction problem such that wall boundary conditions are imposed at top and bottom boundaries. For left and right boundaries, we impose periodic boundary conditions.

Experiments using the matrix dissipation flux [25].

We note that entropy stable wall boundary conditions can also be imposed when using decoupled SBP operators with over-integration as well [11]. As far as the authors know, the stable and high order accurate imposition of such boundary conditions for existing GSBP couplings [13] remains an open problem.

5.4. Inviscid Taylor-Green vortex. We conclude by investigating the behavior of entropy stable Gauss collocation schemes for the inviscid Taylor–Green vortex [37, 3, 10]. This problem is posed on the periodic box $[-\pi, \pi]^3$, with initial conditions

$$\begin{aligned} \rho &= 1 \\ u &= \sin(x_1) \cos(x_2) \cos(x_3), \\ v &= -\cos(x_1) \sin(x_2) \cos(x_3), \\ w &= 0, \\ p &= \frac{100}{\gamma} + \frac{1}{16} (\cos(2x_1) + \cos(2x_2)) (2 + \cos(2x_3)). \end{aligned}$$

The Taylor–Green vortex is used to study the transition and decay of turbulence [38]. In the absence of viscosity, the Taylor–Green vortex develops successively smaller scales as time increases. As a result, the solution is guaranteed to contain under-resolved features after a sufficiently large time. We study the evolution of the kinetic

energy $\kappa(t)$

$$\kappa(t) = \frac{1}{|\Omega|} \int_{\Omega} \rho \mathbf{u} \cdot \mathbf{u} \, d\mathbf{x},$$

as well as the kinetic energy dissipation rate $-\frac{\partial \kappa}{\partial t}$, which is approximated by differencing $\kappa(t)$.

6. Conclusion. Give computational comparison: two point flux evaluations, FLOPS due to matrix operations.

Appendix A. Decoupled SBP operators for general choices of quadrature and basis.

For general choices of quadrature and basis, decoupled projection operators involve a volume quadrature interpolation matrix \mathbf{V}_q , a face quadrature interpolation matrix \mathbf{V}_f , and a quadrature-based L^2 projection matrix \mathbf{P}_q . Let $\{\phi_j\}_{j=1}^{N_p}$ denote a set of N_p basis functions, and let $\{\mathbf{x}_i, \mathbf{w}_i\}_{i=1}^{N_q}$ denote a set of N_q volume quadrature points and weights in d dimensions. Then, $\mathbf{V}_q, \mathbf{V}_f$ are given as

$$\begin{aligned} (\mathbf{V}_q)_{ij} &= \phi_j(\mathbf{x}_i), \quad 1 \leq i, j \leq N_q, \\ (\mathbf{V}_f)_{ij} &= \phi_j(\mathbf{x}_i^f), \quad 1 \leq i \leq N_q, \quad 1 \leq j \leq N_f^f. \end{aligned}$$

These matrices can be used to define the quadrature-based L^2 projection matrix \mathbf{P}_q . Let \mathbf{W} denote the diagonal matrix of quadrature weights. Then,

$$\mathbf{M} = \mathbf{V}_q^T \mathbf{W} \mathbf{V}_q, \quad \mathbf{P}_q = \mathbf{M}^{-1} \mathbf{V}_q^T \mathbf{W}.$$

Let \mathbf{D}^i now denote a modal differentiation matrix with respect to the i th coordinate, which maps coefficients in the basis ϕ_j to coefficients of the i th derivative. By composing this matrix with interpolation and projection matrices, one can define differencing operators $\mathbf{D}_q^i = \mathbf{V}_q \mathbf{D}^i \mathbf{P}_q$ which map values at quadrature points to values of approximate derivatives at quadrature points. It was shown in [11] that $\mathbf{Q}^i = \mathbf{W} \mathbf{D}_q^i$ satisfies a generalized SBP property involving the face interpolation and projection matrices $\mathbf{V}_f, \mathbf{P}_q$.

The decoupled SBP operator \mathbf{Q}_N^i is then given as

$$\mathbf{Q}_N^i = \begin{bmatrix} \mathbf{Q}^i - \frac{1}{2} (\mathbf{V}_f \mathbf{P}_q)^T \mathbf{W}_f \text{diag}(\mathbf{n}_i) \mathbf{V}_f \mathbf{P}_q & \frac{1}{2} (\mathbf{V}_f \mathbf{P}_q)^T \mathbf{W}_f \text{diag}(\mathbf{n}_i) \\ -\frac{1}{2} \mathbf{W}_f \text{diag}(\mathbf{n}_i) \mathbf{V}_f \mathbf{P}_q & \frac{1}{2} \mathbf{W}_f \text{diag}(\mathbf{n}_i) \end{bmatrix}.$$

A straightforward computation shows that \mathbf{Q}_N^i satisfies an SBP property [11]. It is worth noting that the form of \mathbf{Q}_N^i does not depend on the choice of basis. So long as the approximation space spanned by the basis ϕ_j does not change, the domain and range of \mathbf{Q}_N^i depend solely on the choice of volume and surface quadrature points.

A collocation scheme assumes that the number of quadrature points is identical to the number of basis functions. If the solution is represented using degree N Lagrange polynomials at quadrature points, the matrices $\mathbf{V}_q, \mathbf{P}_q$ simplify

$$(\mathbf{V}_q)_{ij} = \delta_{ij}, \quad \mathbf{M} = \mathbf{W}, \quad \mathbf{P}_q = \mathbf{M}^{-1} \mathbf{V}_q^T \mathbf{W} = \mathbf{I}.$$

In summary, the collocation assumption removes the need to interpolate to and from a polynomial space to volume quadrature points within an entropy stable scheme.

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