Efficient computation of Jacobian matrices for entropy stable summation-by-parts schemes

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Abstract

Entropy stable schemes replicate an entropy inequality at the semi-discrete level. These schemes rely on an algebraic summation-by-parts (SBP) structure and a technique referred to as flux differencing. We provide simple and efficient formulas for Jacobian matrices for the semi-discrete systems of ODEs produced by entropy stable discretizations. These formulas are derived based on the structure of flux differencing and derivatives of flux functions, which can be computed using automatic differentiation (AD). Numerical results demonstrate the efficiency and utility of these Jacobian formulas, which are then used in the context of two-derivative explicit time-stepping schemes and implicit time-stepping.

1. Introduction

This paper is concerned with the numerical discretization of systems of nonlinear conservation laws. In particular, we focus on the computation of Jacobian matrices for nonlinear residuals associated with entropy conservative and entropy stable semi-discretizations. Such matrices are useful in the context of implicit time-stepping schemes [1], as well as adjoint-based sensitivity computations and optimization [2, 3].

Entropy stable discretizations mimic a continuous dissipation of entropy for nonlinear conservation laws. Let Ω denote some domain with boundary ∂Ω. Nonlinear conservation laws are expressed as a system of nonlinear partial differential equations (PDEs)

\[ \frac{\partial u}{\partial t} + \sum_{i=1}^{d} \frac{\partial f_i(u)}{\partial x_i} = 0, \quad S(u) \text{ convex}, \quad v(u) = \frac{\partial S}{\partial u}, \quad (1) \]

where \( u \in \mathbb{R}^n \) are the conservative variables, \( f_i \) are nonlinear fluxes, and \( v(u) \) are the entropy variables with respect to the entropy \( S(u) \). By multiplying (1) by the entropy variables, vanishing viscosity solutions [4] of many fluid systems [5, 6] can be shown to satisfy the following entropy inequality

\[ \int_{\Omega} \frac{\partial S(u)}{\partial t} \, dx + \sum_{i=1}^{d} \int_{\partial \Omega} \begin{pmatrix} v^T f_i(u) - \psi_i(u) \end{pmatrix} n_i \leq 0, \quad (2) \]

where \( n_i \) denotes the \( i \)th component of the outward normal vector. The entropy inequality (2) is a statement of stability for nonlinear conservation laws [7, 8].

High order entropy stable schemes (see for example [9, 10, 6, 11, 12, 13, 14]) reproduce this entropy inequality at the semi-discrete level. The resulting methods display significantly improved robustness while retaining high order accuracy [15, 16]. These schemes are based on entropy conservative finite volume fluxes [17], which are extended to high order discretizations through a procedure referred to as flux differencing. These methods have mainly been tested in the context of explicit time-stepping. However, recent works have applied entropy stable methods to both the space-time and implicit settings [18, 19].

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Both space-time and implicit time discretizations require the solution of a system of nonlinear equations. This can be done using Newton’s method, which involves the Jacobian matrix of the nonlinear equations. While it is possible to compute the solution to the nonlinear system without explicitly computing the Jacobian matrix using Jacobian-free Newton-Krylov methods [20, 21], the Jacobian matrix is commonly used to construct preconditioners [1].

In this work, we present efficient formulas for Jacobian matrices of systems resulting from entropy stable formulations. We also show that computing the Jacobian matrix is not significantly more expensive than evaluating the residual of the nonlinear system. Finally, we apply the new Jacobian formulas to both explicit two-derivative and implicit time-stepping schemes.

1.1. On notation

The notation in this paper is motivated by notation in [11, 22]. Unless otherwise specified, vector and matrix quantities are denoted using lower and upper case bold font, respectively. We also denote spatially discrete quantities using a bold sans serif font. Finally, the output of continuous functions evaluated over discrete vectors is interpreted as a discrete vector.

For example, if \(x\) denotes a vector of point locations, i.e., \((x)_i = x_i\), then \(u(x)\) is interpreted as the vector \((u(x))_i = u(x_i)\).

Similarly, if \(u = u(x)\), then \(f(u)\) corresponds to the vector \((f(u))_i = f(u(x_i))\).

Vector-valued functions are treated similarly. For example, given a vector-valued function \(f : \mathbb{R}^n \rightarrow \mathbb{R}^n\) and a vector of coordinates \(x\), \((f(x))_i = f(x_i)\).

2. Jacobian matrix formulas for entropy conservative schemes

For clarity of presentation, we consider first a scalar nonlinear conservation law in one spatial dimension

\[
\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0.
\]

(3)

We assume without loss of generality periodic boundary conditions, which will simplify the presentation of the main results. The generalization to systems of nonlinear conservation laws and higher dimensions is postponed until Section 4.

Let \(f_S(x, y)\) denote a bivariate scalar flux function which is symmetric and consistent. Suppose \(u\) is a vector of nodal values of the solution. Define the vector \(f = f(u)\) approximating the flux derivative \(\frac{\partial f(u)}{\partial x}\) as

\[
f(u) = 2 \left( Q \circ F \right) 1, \quad F_{ij} = f_S(u_i, u_j),
\]

(4)

where \(Q\) is a discretization matrix to be specified later. The simplest entropy stable numerical schemes based on flux differencing discretize (3) via the system of ODEs

\[
M \frac{du}{dt} + f(u) = 0.
\]

(5)

where \(M\) is a diagonal mass (norm) matrix with positive entries. If \(f_S(x, y)\) is entropy conservative (in the sense of [17]) and \(Q\) is skew-symmetric, then the resulting scheme is also discretely entropy conservative. An entropy stable scheme can be constructed from an entropy conservative scheme by adding appropriate terms which dissipate entropy [6, 23, 19].

We are interested in computing the Jacobian matrix \(\frac{\partial f}{\partial u}\). Let \(\text{diag}(x)\) denote the diagonal matrix with the vector \(x\) on the diagonal and let \(\text{diag}(A)\) denote the vector diagonal of \(A\). We then have the following theorem:
Theorem 2.1. Suppose that $Q = \pm Q^T$. Then, the Jacobian matrix of the entropy conservative scheme (4) can be expressed as either

$$\frac{\partial f}{\partial u} = 2 (Q \circ F_y) \pm \text{diag} \left(1^T (2Q \circ F_y)\right)$$
$$\frac{\partial f}{\partial u} = 2 \left(Q \circ F^T_x\right) \pm \text{diag} ((2Q \circ F_x) 1)$$

where the matrices $F_x, F_y$ are

$$(F_x)_{ij} = \frac{\partial f}{\partial x} \bigg|_{u_i, u_j}, \quad (F_y)_{ij} = \frac{\partial f}{\partial y} \bigg|_{u_i, u_j}.$$ 

Proof. We will prove the first formula involving $F_y$. The second formula follows via symmetry and similar steps. By the chain rule,

$$\left(\frac{\partial f}{\partial u}\right)_{ij} = \frac{\partial f_i}{\partial u_j} = \sum_k 2Q_{ik} \frac{\partial f_i}{\partial u_j} f_S(u_i, u_k) = \sum_k 2Q_{ik} \left(\frac{\partial f_i}{\partial x} \bigg|_{u_i, u_k} \frac{\partial u_i}{\partial u_j} + \frac{\partial f_i}{\partial y} \bigg|_{u_i, u_k} \frac{\partial u_k}{\partial u_j}\right)$$

If $i \neq j$, then $\frac{\partial u_i}{\partial u_j} = \delta_{ij} = 0$. Moreover, most terms in the sum over $k$ vanish except for $k = j$. Since $\frac{\partial u_k}{\partial u_j} = 1$, the formula reduces to

$$\frac{\partial f_i}{\partial u_j} = 2Q_{ij} \frac{\partial f_i}{\partial y} \bigg|_{u_i, u_j}.$$ 

When $i = j$, $\frac{\partial u_i}{\partial u_j} = \frac{\partial u_i}{\partial u_i} = 1$, and

$$\frac{\partial f_i}{\partial u_i} = \left(\sum_k 2Q_{ik} \frac{\partial f_i}{\partial x} \bigg|_{u_i, u_k}\right) + 2Q_{ii} \frac{\partial f_i}{\partial y} \bigg|_{u_i, u_i}.$$ 

The term $2Q_{ii} \frac{\partial f_i}{\partial y} \bigg|_{u_i, u_i}$ is the diagonal of the matrix $2(Q \circ F_y)$, and we can simplify the first summation term. By the symmetry of $f_S(x, y)$, we have that

$$\frac{\partial f_i}{\partial y} \bigg|_{x,y} = \frac{\partial f_i}{\partial x} \bigg|_{y,x}$$

Thus, by $Q = \pm Q^T$,

$$\sum_k 2Q_{ik} \frac{\partial f_i}{\partial x} \bigg|_{u_i, u_k} = \sum_k 2Q_{ik} \frac{\partial f_i}{\partial y} \bigg|_{u_i, u_i} = \left(2Q \circ F^T_y\right)_i = \left(\pm 1^T (2Q \circ F_y)\right)_i.$$ 

While we consider only symmetric and skew-symmetric matrices $Q$ in this work, one can use this theorem to compute the Jacobian $\frac{\partial f}{\partial u}$ for arbitrary matrices $Q$ since any real matrix can be decomposed into symmetric and skew parts

$$Q = \frac{1}{2} \left(Q + Q^T\right) + \frac{1}{2} \left(Q - Q^T\right).$$

Two applications of Theorem 2.1 then provide a formula for the Jacobian of (4).
2.1. Computing derivatives of bivariate flux functions

The aforementioned proofs require partial derivatives of flux functions \( f_S(u_L, u_R) \) with respect to at least one argument. This can be done by hand for simple fluxes. For example, for the Burgers’ equation, the flux and its derivative are

\[
 f_S(u_L, u_R) = \frac{1}{6} (u_L^2 + u_L u_R + u_R^2), \quad \frac{\partial f_S}{\partial u_R} = \frac{1}{6} (u_L + 2u_R).
\]

However, this procedure can become cumbersome for complex or piecewise-defined flux functions such as the logarithmic mean \([24, 25]\). This can be avoided by using Automatic Differentiation (AD) \([26]\). AD is distinct from both symbolic differentiation and finite difference approximations in that it does not return an explicit expression, but constructs a separate function which evaluates the derivative accurately up to machine precision.

In this work, we utilize the Julia implementation of forward-mode automatic differentiation provided by \texttt{ForwardDiff.jl} \([27]\). The procedure is remarkably simple: given some flux function \( f(x, y) \), \texttt{ForwardDiff.jl} returns the derivative with respect to either \( x \) or \( y \) as another function. For example, defining the function \( \frac{\partial f}{\partial y} \big|_{x,y} \) is a one-line operation:

\[
 dfdy(x,y) = \text{ForwardDiff.derivative}(y->f(x,y),y)
\]

\texttt{ForwardDiff.jacobian} is the analogous routine for computing Jacobians of vector-valued flux functions. This simple API utilizes the flexible Julia type system \([28]\).

Automatic differentiation can be directly applied to \( f(u) \) to compute the Jacobian matrix. However, because AD scales with the number of inputs and outputs, the cost of applying AD directly to \( f(u) \) increases as the discretization resolution increases. In contrast, using the approach in this paper, AD is applied only to the flux function, which has a small fixed number of inputs and outputs which are independent of the discretization resolution. As a result, the cost of evaluating derivatives of the flux function is roughly the same as the cost of evaluating the flux function itself and entries of the Jacobian matrix can be computed for roughly the same cost as a single evaluation of the nonlinear flux \( f(u) \). Moreover, when computing the Jacobian matrix, the formula in Theorem 2.1 makes it simpler to directly take advantage of sparsity in \( Q \) without having to perform graph coloring \([29]\).

3. Examples of discretization matrices which appear in entropy conservative numerical schemes

In this section, we give some examples of matrices \( Q \) which appear in entropy stable numerical discretizations. We assume periodicity, which corresponds to a skew-symmetric structure for \( Q \). Non-periodic domains are treated later.

3.1. Finite volume methods

The spatial discretization for a finite volume scheme can be reformulated in terms of (4) \([30]\). Suppose that the 1D interval \([-1, 1]\) is decomposed into \( K \) non-overlapping elements of size \( h \). An entropy conservative finite volume scheme is given as

\[
 \frac{du_1}{dt} + \frac{f_S(u_2, u_1) - f_S(u_1, u_K)}{h} = 0
\]

\[
 \frac{du_i}{dt} + \frac{f_S(u_{i+1}, u_i) - f_S(u_i, u_{i-1})}{h} = 0, \quad i = 2, \ldots, K - 1,
\]

\[
 \frac{du_K}{dt} + \frac{f_S(u_1, u_K) - f_S(u_K, u_{K-1})}{h} = 0,
\]

\[\text{1} \text{In practice, derivative and Jacobian functions are initialized with information about the size and data type of the input to ensure type stability in Julia.}\]
where \( u_i \) denotes the average value of the solution on each element and \( f_S \) is an entropy conservative flux. Let \( M = h I \) and let \( Q \) be the periodic second-order central difference matrix

\[
Q = \frac{1}{2} \begin{bmatrix}
0 & 1 & \ldots & -1 \\
-1 & 0 & 1 & \\
& -1 & 0 & 1 \\
1 & \ldots & -1 & 0
\end{bmatrix}.
\]

An entropy conservative finite volume scheme is then equivalent to

\[
\frac{d u}{d t} + 2 (Q \circ F) \mathbf{1} = 0, \quad F_{ij} = f_S(u_i, u_j)
\]

where \( u = [u_1, \ldots, u_K]^T \) is the vector of solution values.

3.2. Multi-block summation-by-parts finite differences and discontinuous Galerkin spectral element methods

We consider next a multi-element summation-by-parts (SBP) finite element discretization [31, 32]. Suppose again that a one-dimensional domain \( \Omega \) is decomposed into \( K \) non-overlapping elements \( D^k \) of size \( h \). Let \( M \) and \( Q \in \mathbb{R}^{N_p \times N_p} \) denote diagonal mass (norm) and nodal differentiation matrices such that \( M^{-1} Q \) approximates the first derivative on a reference interval and is exact for polynomials up to degree \( N \). The operators \( M, Q \) satisfy an SBP property if

\[
Q + Q^T = B, \quad B = \begin{bmatrix} -1 & 0 & \ldots & 0 \\
0 & \ddots & \ddots & \ddots \\
& & 0 & \ddots \\
& & & 1 \end{bmatrix}.
\] (5)

We note that nodal discontinuous Galerkin spectral element (DG-SEM) discretizations [33] also fall into a SBP framework [34] and are thus also included in this framework.

These matrices can be used to construct entropy conservative high order discretizations. Let \( J = h/2 \) be the Jacobian of the mapping from the reference element \([-1, 1]\) to a physical interval of size \( h \) and let \( F_{ij} = f_S(u_i,k, u_j,k) \) denote the matrix of flux interactions between different nodes on the element \( D^k \). A local formulation on the element \( D^k \) is given by

\[
J_k M \frac{d u_k}{d t} + 2 (Q \circ F^k) \mathbf{1} + B (f^* - f(u_k)) = 0,
\]

\[
f^* = \begin{cases} f_S(u_{1,k}^+, u_{1,k}) \\
0 \\
\vdots \\
0 \\
0 \\
f_S(u_{N_p,k}^+, u_{N_p,k}) \end{cases}.
\] (6)

where \( u_{1,k}^+, u_{N_p,k}^+ \) denote the exterior values of \( u_{1,k}, u_{N_p,k} \) on neighboring elements. Assuming that the elements are ordered from left to right in ascending order, for interior element indices \( 1 < k < K \), these are given by

\[
u_{1,k}^+ = u_{N_p,k-1}, \quad u_{N_p,k}^+ = u_{1,k+1}.
\]

In other words, the first node on \( D^k \) is connected to the last node on the previous element, and the last node on \( D^k \) is connected to the first node on the next element.
For periodic boundary conditions this local formulation can be understood as inducing a global skew-symmetric matrix. To show this, we first use the SBP property to rewrite (6) in a skew-symmetric form

$$J_k M \frac{d u_k}{d t} + \left( \left( Q - Q^T \right) \circ F^k \right) 1 + B f^* = 0.$$

We now define a global vector $u_\Omega = [u_1, u_2, \ldots, u_K]^T$. Let the global flux matrix be defined as

$$F = \begin{bmatrix} F_{11} & \cdots & F_{1K} \\ \vdots & \ddots & \vdots \\ F_{K1} & \cdots & F_{KK} \end{bmatrix}, \quad (F_{k1,k2})_{ij} = f_S(u_{k1,i}, u_{k2,j}).$$

The blocks of the matrix $F$ capture flux interactions between solution values at different nodes and elements. The local formulations can now be concatenated into a single skew-symmetric matrix

$$M_\Omega \frac{d u_\Omega}{d t} + 2 \left( Q_\Omega \circ F \right) 1 = 0,$$

where $M_\Omega$ is the block-diagonal matrix with blocks $J_k M$, and

$$Q_\Omega = \frac{1}{2} \begin{bmatrix} S & B_R & -B_L \\ -B_L & S & B_R \\ B_R & -B_L & S \end{bmatrix}, \quad S = \left( Q - Q^T \right).$$

where the matrices $B_L, B_R$ are zeros except for a single entry

$$B_L = \begin{bmatrix} 1 \\ \vdots \\ 0 \end{bmatrix}, \quad B_R = B_L^T = \begin{bmatrix} 0 \\ \vdots \\ 1 \end{bmatrix} \quad (9)$$

The matrix $Q_\Omega$ can be considered a high order generalization of the finite volume matrix (5). Similar “global SBP operator” approaches were used to construct simultaneous approximation (SBP-SAT) interface coupling terms in [11, 36, 22].

The generalization to higher dimensional domains and curved geometric mappings is straightforward, but notationally much more complicated. The construction of skew-symmetric global matrices $Q_\Omega$ on curved meshes follows from approaches detailed in [9, 11, 12, 37, 36, 35, 19]. For conciseness, we omit the assembly of multi-dimensional global differentiation matrices in this work, but note that the assembly of multi-dimensional DG matrices is discussed in detail elsewhere [1, 38, 39].

4. Systems of conservation laws

In this section, we extend the Jacobian formulas of Theorem 2.1 from scalar nonlinear conservation laws to an $n \times n$ system of conservation laws. Let $f_S(u_L, u_R) : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ denote an entropy conservative flux function for a 1D system of conservation laws. We first formulate a system of ODEs by modifying the definition of the arrays and matrices in (8).

Let $u_\Omega$ denote a vector of vectors

$$u_\Omega = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}, \quad u_i = \begin{bmatrix} u_{i,1} \\ u_{i,2} \\ \vdots \\ u_{i,K} \end{bmatrix}, \quad u_{i,k} = \begin{bmatrix} u_{i,k,1} \\ u_{i,k,2} \\ \vdots \\ u_{i,k,N_p} \end{bmatrix} \quad (10)$$
for \( \ell = 1, \ldots, n, k = 1, \ldots, K \) and \( j = 1, \ldots, N_p \). Here, \( u_{i,k,j} \) denotes the \( j \)th degree of freedom for the \( \ell \)th component of the solution on the \( k \)th element. Let \((k_1,j_1)\) and \((k_2,j_2)\) be multi-indices which correspond to row and columns indices of a matrix, respectively. We now define the flux matrix \( F \) as the \( n \times n \) block diagonal matrix containing flux interactions between different nodes

\[
F = \begin{bmatrix}
F_1 & \cdots & F_n \\
\cdots & \ddots & \cdots \\
F_n & \cdots & F_1
\end{bmatrix}, \quad (F_\ell)(k_1,j_1),(k_2,j_2) = (f_S(u_{i,k_1,j_1},u_{i,k_2,j_2}))_\ell. \tag{11}
\]

where \( u_{i,k,j} \) denotes the vector containing all solution components at the \( k \)th element and \( j \)th node, and each entry of the block \( F_\ell \) for \( \ell = 1, \ldots, n \) corresponds to the \( \ell \)th component of the vector-valued flux evaluated at solution states \( u_{i,k_1,j},u_{i,k_2,j} \).

Let \( M_\Omega,Q_\Omega \) denote the global mass and differentiation matrices in (8). Then, an entropy conservative scheme is given by

\[
(l_n \otimes M_\Omega) \frac{d u_\Omega}{dt} + 2 ((l_n \otimes Q_\Omega) \circ F) 1 = 0.
\]

where \( l_n \in \mathbb{R}^n \) is the \( n \times n \) identity matrix.

We now provide Jacobian matrix formulas for systems of nonlinear conservation laws. The proofs are straightforward extensions of the proof of Theorem 2.1 to the vector-valued case, and we omit them for conciseness. The right hand side function \( f(u) \) for systems can be rewritten as

\[
f(u) = 2 ((l_n \otimes Q_\Omega) \circ F) 1 = 2 \begin{bmatrix}
(Q_\Omega \circ F_1) \\
\vdots \\
(Q_\Omega \circ F_n)
\end{bmatrix} 1.
\]

Then, the Jacobian matrix is

\[
\frac{\partial f}{\partial u} = \begin{bmatrix}
\partial F_{1,u_1} & \cdots & \partial F_{1,u_n} \\
\vdots & \ddots & \vdots \\
\partial F_{n,u_1} & \cdots & \partial F_{n,u_n}
\end{bmatrix} \tag{12}
\]

where each Jacobian block \( \partial F_{i,u_j} \) is evaluated as in Theorem 2.1

\[
\partial F_{i,u_j} = 2 (Q_\Omega \circ F_{i,u_j}) \pm \text{diag} \left( 1^T (2Q_\Omega \circ F_{i,u}) \right)
\]

\[
\partial F_{i,u_j} = 2 (Q_\Omega \circ F_{u,j})^T \pm \text{diag} \left( 2Q_\Omega \circ F_{u,j} \right) 1.
\]

for \( Q_\Omega = \pm Q_\Omega^T \). Here, the flux matrix \( F_{i,u_j} \) is evaluated via one of two formulas

\[
(F_{i,u_j})_{(j_1,k_1),(j_2,k_2)} = \frac{\partial (f_S)}{\partial u_{R,j}} \bigg|_{u_{i,k_1,j_1},u_{i,k_2,j_2}}
\]

\[
(F_{u,j})_{(j_1,k_1),(j_2,k_2)} = \frac{\partial (f_S)}{\partial u_{L,j}} \bigg|_{u_{i,k_1,j_1},u_{i,k_2,j_2}}.
\]

where \( \frac{\partial (f_S)}{\partial u_{L,j}}, \frac{\partial (f_S)}{\partial u_{R,j}} \) denote the derivatives of the \( i \)th component of the flux \( f_S(u_L,u_R) \) with respect to the \( j \)th solution component of \( u_L,u_R \). Thus, each entry of the block \( F_{i,u_j} \) corresponds to an entry of the Jacobian (with respect to \( u_L \) or \( u_R \)) of \( f_S(u_L,u_R) \) and an entry of the global differentiation matrix \( Q_\Omega \).

Remark 1. An alternative ordering of the degrees of freedom [11] yields a Jacobian matrix with a more compact bandwidth. A smaller matrix bandwidth can also be achieved by precomputing bandwidth-minimizing row and column permutations using the reverse Cuthill-McKee algorithm [40].
5. Extension to entropy stable (dissipative) schemes

We now consider entropy stable schemes, which include entropy dissipation terms to produce a semi-discrete dissipation (rather than conservation) of entropy. These can correspond either to physical or artificial viscosity mechanisms [41, 23] or numerical interface dissipation [42]. Because Jacobian matrices for artificial viscosity mechanisms have been discussed in more detail in the time-implicit literature [43] we focus instead on numerical interface dissipation.

Let \( d_S(u_L, u_R) \) be an entropy dissipative anti-symmetric flux such that
\[
d_S(u_L, u_R) = -d_S(u_R, u_L), \quad (v_L - v_R)^T d_S(u_L, u_R) \geq 0.
\]
Note that the anti-symmetry of \( d_S \) implies that \( d_S(u, u) = 0 \). Fluxes which fall into this category include the Lax-Friedrichs flux
\[
d_S(u_L, u_R) = \frac{|\lambda|}{2} (u_L - u_R), \quad \lambda = \text{estimate of maximum wavespeed},
\]
as well as HLLC fluxes [6] and matrix dissipation fluxes [42].

5.1. Scalar dissipative fluxes

We will begin by considering scalar dissipative fluxes \( d_S(u_L, u_R) \) and dissipation terms of the form
\[
d(u) = (B \circ D) 1
\]
where \( B \) is a symmetric positive semi-definite matrix and the entries of \( D_{ij} = d_S(u_i, u_j) \) correspond to evaluations of the dissipative flux. For the high order DG-SBP discretizations of periodic domains described in (7), \( B_{\Omega} \) is the matrix
\[
B = \frac{1}{2} \begin{bmatrix}
B_R & B_R & B_L \\
B_L & B_R & B_L \\
B_R & B_L & B_R \\
\end{bmatrix}
\]
where \( B_L, B_R \) are defined as in (9).

To compute the Jacobian of this term, we can note that Theorem 2.1 assumes that the discretization matrix is skew-symmetric (or symmetric), while the flux matrix is symmetric. Here, the orders are reversed — the flux matrix \( D \) is now skew-symmetric, while the discretization matrix \( B_{\Omega} \) is symmetric. Thus, repeating the steps of the proof of Theorem 2.1, one can show that the Jacobians of the dissipative term can be computed using one of two formulas.

\[\text{Theorem 5.1.} \quad \frac{\partial d}{\partial u} = -(B \circ D_x^T) + \text{diag} \left( B \circ D_x^T 1 \right), \quad \frac{\partial d}{\partial u} = (B \circ D_y) - \text{diag} \left( D_x^T (B \circ D_y) \right)\]

where the matrices \( D_x, D_y \) are
\[
(D_x)_{ij} = \left. \frac{\partial d_S}{\partial u_L} \right|_{u_i, u_j}, \quad (D_y)_{ij} = \left. \frac{\partial d_S}{\partial u_R} \right|_{u_i, u_j}.
\]
Proof. We will prove the second formula in (14) involving $D_S$ using the same approach as the proof of Theorem 2.1. The proof of the first formula results from the fact that $D_S = -D_L^T$ by the anti-symmetry of $d_S(u_L, u_R)$. Applying the chain rule yields

$$\frac{\partial d_i}{\partial u_j} = \sum_k B_{ik} \left( \left. \frac{\partial d_S}{\partial x} \right|_{u_i, u_k} \frac{\partial u_i}{u_j} + \left. \frac{\partial d_S}{\partial y} \right|_{u_i, u_k} \frac{\partial u_k}{u_j} \right)$$

If $i \neq j$, then $\frac{\partial u_i}{u_j} = 0$ and the sum reduces to the single term $k = j$

$$\frac{\partial d_i}{\partial u_j} = B_{ij} \left. \frac{\partial f_S}{\partial y} \right|_{u_i, u_j}.$$}

For $i = j$, $\frac{\partial u_i}{u_j} = 1$. Using the symmetry of $B$ and anti-symmetry of $d_S$ yields

$$\frac{\partial d_i}{\partial u_i} = \left( \sum_k B_{ik} \left. \frac{\partial d_S}{\partial x} \right|_{u_i, u_k} \right) + B_{ii} \left. \frac{\partial d_S}{\partial y} \right|_{u_i, u_i} = \left( \sum_k B_{ik} \left. \frac{\partial d_S}{\partial y} \right|_{u_i, u_k} \right) + B_{ii} \left. \frac{\partial d_S}{\partial y} \right|_{u_i, u_i}.$$} \[ \square \]

5.2. Vector-valued dissipative fluxes

For a vector-valued dissipative flux, the dissipative contribution is

$$d(u) = \begin{bmatrix} (B \circ D_1) \\ \vdots \\ (B \circ D_n) \end{bmatrix} 1,$$

where each matrix block $(D_i)_{(j_1,k_1),(j_2,k_2)} = (d_S(u_{j_1}, u_{j_2}, u_{k_1}, u_{k_2}))_i$ corresponds to the $i$th component of the dissipative flux, where $u$ is ordered as in (10). Then, the Jacobian of $d(u)$ yields the following block matrix

$$\frac{\partial d}{\partial u} = \begin{bmatrix} \partial D_{1,u_1} & \cdots & \partial D_{1,u_n} \\ \vdots & \ddots & \vdots \\ \partial D_{n,u_1} & \cdots & \partial D_{n,u_n} \end{bmatrix}$$

(15)

where each Jacobian block $\partial D_{i,u_j}$ is evaluated as in (14) using one of two formulas

$$\partial D_{i,u_j} = (B \circ D_{i,u_j}) - \text{diag} \left( (B \circ D_{i,u_j}) \right),$$

$$\partial D_{i,u_j} = -(B \circ D_{u_i,j}) + \text{diag} \left( (B \circ D_{u_i,j}) \right).$$

where the dissipative flux matrices $D_{i,u_j}, D_{u_i,j}$ are defined in terms of entries of the Jacobian of $d_S$

$$(D_{i,u_j})_{(j_1,k_1),(j_2,k_2)} = \left. \frac{\partial (d_S)}{\partial u_{R,j}} \right|_{u_{j_1},u_{j_2}} \left. \frac{\partial (d_S)}{\partial u_{R,j}} \right|_{u_{k_1},u_{k_2},j_2},$$

$$(D_{u_i,j})_{(j_1,k_1),(j_2,k_2)} = \left. \frac{\partial (d_S)}{\partial u_{L,j}} \right|_{u_{j_1},u_{j_2}} \left. \frac{\partial (d_S)}{\partial u_{L,j}} \right|_{u_{k_1},u_{k_2},j_2}.$$

Remark 2. If the derivative of $d_S$ with respect to its second argument $u_R$ is used to compute the dissipative flux matrices, then the structure of the dissipative Jacobian is identical to the structure of the entropy conservative Jacobian (12). Thus, given discretization matrices $Q_{ij}, B_{ij}$ and functions which evaluate derivatives of flux functions $f_S$, $d_S$ with respect to their second arguments, the same routine can be used to compute both the entropy conservative and dissipative Jacobians.
6. Non-collocated schemes: hybridized SBP operators, entropy projection, over-integration

Most entropy stable schemes rely on “collocated” SBP operators (where the mass matrix $M_\Omega$ is diagonal) constructed using nodal sets which include boundary nodes [6, 11]. However, in certain cases energy and entropy stable SBP schemes constructed using non-diagonal mass matrices [12, 30] and more general nodal sets [44, 45, 46, 36] achieve higher accuracy than SBP schemes built on nodal sets which include boundary nodes. We discuss how to extend Jacobian formulas to “modal” formulations for entropy conservative schemes (the extension to entropy stable schemes is similar).

6.1. “Modal” entropy conservative schemes

We now assume that the solution is represented using a “modal” expansion

$$u(x, t) \approx \sum_{j=1}^{N_p} \tilde{u}_{k,j}(t) \phi_i(x),$$

where $\tilde{u}_{k,j}$ denotes the coefficients of the solution on an element $D_k$. We assume two sets of quadrature points: volume quadrature points and weights, $\{w_i, x_{q,i}\}_{i=1}^{N_q}$, and surface quadrature points, $\{w_f,i, x_{f,i}\}_{i=1}^{N_f}$. We assume both quadrature rules are exact for certain classes of integrands as detailed in [35, 30]. Evaluating $u(x, t)$ at quadrature points requires multiplication by an interpolation matrix

$$V_{ij} = \phi_j(x_i), \quad i = 1, \ldots, N_q, \quad j = 1, \ldots, N_p$$

We can similarly define mass and projection matrices $M, P$

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

where $W$ is a diagonal matrix whose entries are the quadrature weights $w_i$. We also define a face interpolation matrix

$$E = V_f P$$

which evaluates the solution at face quadrature points given values at volume quadrature points. Finally, we define the matrix $V_h$ as the mapping between local coefficients $\tilde{u}_k$ and the combined vector of volume and surface quadrature points

$$V_h = \begin{bmatrix} V \\ V_f \end{bmatrix}.$$  

These matrices are involved in the application of hybridized SBP operators (originally referred to as decoupled SBP operators) [12, 47]. We present the main ideas in a 1D setting and refer the reader to [11, 12, 35] for details on multi-dimensional settings.

Given some modal weak differentiation matrix $\hat{Q}$ which acts on the basis coefficients $\tilde{u}_k$, we define a nodal differentiation matrix $Q = P^T \hat{Q} P$. Then we can define a hybridized SBP operator as

$$Q_h = \frac{1}{2} \begin{bmatrix} Q - Q^T E^T B & E^T B \\ -E B & B \end{bmatrix}, \quad B = \begin{bmatrix} -1 \\ 1 \end{bmatrix}.$$  

The operator $Q_h$ can be used to approximate coefficients of the derivative in the basis $\phi_i(x)$. Let $f(u)$ denote some function of $u(x)$, and let $\tilde{f}$ denote the basis coefficients of $u(x)$. Then,

$$\frac{\partial f(u)}{\partial x} \approx \sum_j \hat{f}_j \phi_j(x), \quad \hat{f} = M^{-1} V^T_h Q_h (V_h \tilde{u}).$$
We now construct global matrices for the multi-element (periodic) case. We begin by concatenating the local coefficients $\hat{u}_{k,i}$ into a global coefficient vector $\hat{u}_\Omega$. We also introduce boundary matrices $B, B_L,$ and $B_R$ which enforce coupling between different elements and are defined as

$$B_L = \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}, \quad B_R = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} -1 & 1 \\ 0 & 1 \end{bmatrix}.$$ 

In the multi-dimensional case, the entries of $B_L, B_R$ correspond instead to outward normals $[11, 12]$.

We can also adapt $Q_h$ to construct a globally skew-symmetric differentiation matrix (see also [36]). Define the matrix $S = Q - Q^T$ and define $Q_\Omega$ as the global block matrix

$$Q_\Omega = \frac{1}{2} \begin{bmatrix} S & E^T B & -B_L \\ -B_L & B_R & -BE \\ E^T B & -BE & -B_L \\ -B_L & -BE & S \\ B_R & -BE & -B_L \\ -BE & -B_L & S \end{bmatrix}.$$ 

We abuse notation and redefine $V, E, P$ and $V_h$ as global interpolation, projection, and extrapolation matrices

$$V \rightarrow I_K \otimes V, \quad P \rightarrow I_K \otimes P, \quad E \rightarrow I_K \otimes E, \quad V_h \rightarrow I_K \otimes V_h.$$ 

Finally, we assume that the global solution $u(x,t) \in \mathbb{R}^n$ is vector-valued, and order the solution coefficients as in Section 4.

It was shown in [13, 12] that when either the mass matrix is non-diagonal or the nodal set does not contain appropriate boundary points, it is necessary to perform an entropy projection (or extrapolation [47]) step to ensure discrete entropy stability. Let $v(u)$ denote the entropy variables as a function of the conservative variables, and let $u(v)$ denote the inverse mapping. We define the entropy projected variables $\tilde{u}_\Omega$ as

$$\tilde{u}_\Omega = u(\mathbf{V}_h \mathbf{P} v(\mathbf{V}_h \hat{u}_\Omega)).$$ (16)

Let $F$ again denote the block-diagonal flux matrix in (11). We evaluate each flux block $F_\ell$ using the entropy projected variables

$$(F_\ell)_{(k_1,j_1),(k_2,j_2)} = (f_S (\tilde{u}_{k_1,j_1, k_2,j_2}))_\ell.$$ (17)

Then, an entropy conservative method is given by

$$(I_n \otimes M_\Omega) \frac{d\tilde{u}_\Omega}{dt} + 2 (I_n \otimes \mathbf{V}_h)^T \left( (I_n 1_n^T \otimes Q_\Omega) \circ F \right) 1 = 0.$$ 

where $I_n$ is the $n \times n$ identity matrix and $1_n$ denotes the length $n$ vector of all ones.

6.2. Jacobian matrices for modal entropy stable schemes

We redefine the nonlinear term as

$$f(\tilde{u}) = 2 (I_n \otimes \mathbf{V}_h)^T \left( (I_n 1_n^T \otimes Q_\Omega) \circ F \right) 1.$$ 

where the flux matrix $F$ is computed using the entropy projected conservative variables (16) via (17). Let $\frac{\partial u}{\partial v}$ and $\frac{\partial v}{\partial u}$ denote Jacobians of the conservative variables with respect to the entropy variables and vice versa.
These have been explicitly derived for several equations (for example, the Jacobians for the compressible Navier-Stokes equations are given in [5]).

We can compute the Jacobian of \( f(\bar{u}) \) via the chain rule. We assume a scalar equation \( n = 1 \) for simplicity, and motivate our approach by considering an entry \( i \neq j \) of the Jacobian

\[
\left( \frac{\partial f}{\partial \bar{u}_{i}} \right)_{ij} = 2 \mathbf{V}_h^T \frac{\partial}{\partial (\bar{u}_i)} \left( (\mathbf{Q}_\Omega \circ \mathbf{F}) \mathbf{1} \right)_i.
\]

We focus on the latter term \( \frac{\partial}{\partial \bar{u}_i} (\mathbf{Q}_\Omega \circ \mathbf{F}) \mathbf{1} \)

\[
\left( \frac{\partial}{\partial \bar{u}_i} \left( \mathbf{Q}_\Omega \circ \mathbf{F} \right) \mathbf{1} \right)_{ij} = \frac{\partial}{\partial \bar{u}_{i,j}} \left( \sum_k (\mathbf{Q}_\Omega)_{ik} f_S (\bar{u}_i, \bar{u}_k) = \sum_k (\mathbf{Q}_\Omega)_{ik} \frac{\partial f_S}{\partial y} \bigg|_{\bar{u}_i, \bar{u}_k} \frac{\partial \bar{u}_j}{\partial \bar{u}_{i,j}} \right)
\]

We observe that the term \( \frac{\partial \bar{u}_i}{\partial \bar{u}_{i,j}} \) does not disappear as it did in the proof of Theorem 2.1. We thus treat the Jacobian matrix in two parts. First, we define the “unassembled” Jacobian matrix \( \frac{\partial f}{\partial \bar{u}} \) as

\[
\left( \frac{\partial f}{\partial \bar{u}} \right)_{ij} = (\mathbf{Q}_\Omega)_{ij} \frac{\partial f_S}{\partial y} \bigg|_{\bar{u}_i, \bar{u}_j} = (\mathbf{Q}_\Omega \circ \mathbf{F})_{ij}.
\]

The construction of \( \frac{\partial \bar{u}_i}{\partial \bar{u}_{i,j}} \) for systems \( n > 1 \) is carried out using the procedure described in Section 4. Let \( \bar{v} \) denote the projected entropy variables evaluated at volume quadrature points

\[
\bar{v} = \mathbf{V}_h \mathbf{P} \left( \mathbf{V} \bar{u}_\Omega \right).
\]

The vector \( \frac{\partial \bar{u}}{\partial \bar{u}_\Omega} \) can be further expanded as

\[
\frac{\partial \bar{u}}{\partial \bar{v}_\Omega} = \left[ \begin{array}{c}
\frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_1} \\
\vdots \\
\frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_k}
\end{array} \right], \quad \frac{\partial \bar{u}}{\partial \bar{v}_\Omega} = \left[ \begin{array}{c}
\frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_1} \\
\vdots \\
\frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_k}
\end{array} \right],
\]

where the Jacobian matrices for the maps between conservative and entropy variables are block diagonal matrices given by

\[
\frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_1} = \left[ \begin{array}{c}
\frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_1} \\
\vdots \\
\frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_k}
\end{array} \right], \quad \frac{\partial \bar{u}}{\partial \bar{v}_\Omega} = \left[ \begin{array}{c}
\frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_1} \\
\vdots \\
\frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_k}
\end{array} \right],
\]

where the local block \( \frac{\partial \bar{u}}{\partial \bar{v}} \bigg|_{\bar{u}_{j,k}} \) is the Jacobian matrix \( \frac{\partial \bar{u}}{\partial \bar{v}} \) evaluated at the \( j \)th nodal solution value \( \bar{u}_{j,k} \) on the \( k \)th element.

Let \( N_p, N_q \), and \( N_f \) denote the number of total basis functions, quadrature points, and face quadrature points respectively, and define \( N_{\text{total}} = N_q + N_f \). The structure and dimensions of matrices involved in constructing the “assembled” Jacobian matrix are illustrated as follows:

\[
\frac{\partial f}{\partial \bar{u}_\Omega} = \left[ \begin{array}{c|c|c|c}
\mathbf{V}_h^T & \mathbf{Q}_\Omega \circ \frac{\partial \bar{u}}{\partial \bar{v}} & \mathbf{V}_h \mathbf{P} & \frac{\partial \bar{u}}{\partial \bar{v}} \mathbf{V}_h \bar{u}_\Omega
\end{array} \right]
\]

\[
\left( (N_{\text{total}} \times N_{\text{total}}) \right), \quad \left( (N_{\text{total}} \times N_{\text{total}}) \right), \quad \left( (N_{\text{total}} \times N_{\text{total}}) \right), \quad \left( (N_q \times N_q) \right), \quad \left( (N_q \times N_p) \right)
\]

“Unassembled” and “assembled” Jacobian matrices (18) and (20) for Burgers’ equation are shown in Figure 1. We note that the structure of these matrices becomes simplified under common assumptions
for entropy stable discretizations. The most common assumptions are either “collocated volume nodes” or “collocated volume and surface nodes” [48]. When volume nodes are collocated, the solution is represented using a nodal Lagrange basis constructed using $N_q = N_p$ volume quadrature nodes. When surface nodes are collocated, the surface quadrature points are also a subset of the volume quadrature nodes [34, 6].

If only volume nodes are collocated [36], then $V = I$. If both volume and surface nodes are collocated, the system reduces to the simplified system described in Section 4 using the fact that $\frac{\partial u}{\partial v} = (\frac{\partial v}{\partial u})^{-1}$.

7. Numerical experiments

In this section, we compare the computational efficiency of the formulas derived in this paper with other methods for computing the Jacobian. Additionally, we apply these Jacobian formulas to two-derivative time-stepping methods [49] and time-implicit discretizations.

7.1. Comparisons of computational cost

We first compare the cost of computing the Jacobian matrix using the formulas in this paper to other approaches. All computations are performed on a 2019 Macbook Pro with a 2.3 GHz 8-Core Intel Core i9 processor using Julia version 1.4 and all timings are computed using the BenchmarkTools.jl package [50].

First, we compare the cost of evaluating a flux function $f_S(u_L, u_R)$ to the cost of computing its derivative using ForwardDiff.jl. We consider three flux functions: an energy stable flux for Burgers’ equation, a rational kernel, and the logarithmic mean

$$f_S(u_L, u_R) = \begin{cases} \frac{1}{6} \left(u_L^2 + u_L u_R + u_R^2\right) & \text{Burgers’ flux} \\ (u_L + u_R)^{-1} & \text{rational kernel} \\ \log u_L - \log u_R & \text{logarithmic mean} \end{cases}$$

The logarithmic mean is computed using the numerically stable expansion of [25] with $\gamma = 1.4$. We evaluate both the function and derivative for two random vectors of values $u_L, u_R \in \mathbb{R}^{10000}$ (for the logarithmic mean, the entries of the random vectors are set to be positive).

---

[2] This definition refers to discretizations which utilize an explicit basis. For entropy stable SBP discretizations, volume nodes are typically collocated by construction. This is possible because nodal degrees of freedom for SBP discretizations do not necessarily correspond to a nodal basis.
The evaluation of the Burgers’ flux takes 7.087 microseconds, while the derivative takes 7.063 microseconds to evaluate. The rational kernel takes 7.132 microseconds to evaluate, while its derivative takes 13.593 microseconds to evaluate. Finally, the logarithmic mean takes 129.254 microseconds to evaluate, while its derivative takes 161.322 microseconds to evaluate. In each case, the cost of evaluating the derivative of the flux function is at most $1.9 \times$ the cost of evaluating the function. The cost of computing the Jacobian using ForwardDiff.jl scales similarly. Because the steps are trivially parallelizable with high arithmetic intensity, the use of multi-threading or GPU acceleration is not expected to significantly change the relative costs.

Next, we compare the cost of computing both the full Jacobian and a Jacobian-vector product using the formulas in Theorem 2.1 and competing approaches. Let $f_S(u_L, u_R)$ denote the scalar flux Burgers’ flux, and define

$$ f(u) = (Q \circ F)\mathbf{1}, \quad F_{ij} = f_S(u_i, u_j), $$

where $Q \in \mathbb{R}^{N,N}$ is a dense randomly generated skew-symmetric matrix. We compute the Jacobian matrix using the formula from Theorem 2.1 (referred to as “Formula from Theorem 2.1” in Table 1), with $\frac{d f_S}{d u_R}$ computed using both the analytical formula and automatic differentiation, which are tagged as “(analytic)” and “(AD)” in Table 1. We also compute the full Jacobian matrix directly using ForwardDiff.jl (referred to as “Automatic differentiation” in Table 1). We also compute the Jacobian matrix using the FiniteDiff.jl toolkit within the DifferentialEquations.jl framework [51], which computes the Jacobian matrix efficiently using cached in-place function evaluations and finite difference approximations (referred to as “finite differences” in Table 1). Finally, we provide timings for evaluating $f(u)$ for reference. Implementations of both $f(u)$ and its Jacobian are optimized for performance in Julia.\(^{3}\)

|                | N = 10  | N = 25  | N = 50  |
|----------------|--------|--------|--------|
| Automatic differentiation | 5.666  | 60.388 | 373.633 |
| Finite differences      | 1.429  | 17.324 | 125.894 |
| Formula from Theorem 2.1 (analytic) | .209   | 1.005  | 3.249  |
| Formula from Theorem 2.1 (AD)     | .210   | 1.030  | 3.259  |
| Evaluation of $f(u)$ (for reference) | .120  | .623   | 2.403  |

Table 1: Timings for the computation of $f(u)$ in (21) and various methods of computing the full Jacobian $\frac{d f}{d u}$ using the scalar Burgers’ flux $f_S(u_L, u_R) = (u_L^2 + u_L u_R + u_R^2)/6$ (times in microseconds).

We observe that the cost of evaluating the full Jacobian matrix using the formula of Theorem 2.1 is 1-2 orders of magnitude less expensive than automatic differentiation or finite differences applied directly to the nonlinear term $f(u)$. These results highlight the fact that automatic differentiation is most efficient for functions with a small number of inputs and outputs, which the formulas in Theorem 2.1 exploit.

Because the number of flux evaluations required to evaluate $f(u)$ is comparable to the number of AD function evaluations required to evaluate the Jacobian matrix, the cost of evaluating the full Jacobian matrix is proportional to the cost of directly evaluating $f(u)$. Here, the constant of proportionality is roughly equal to the ratio of the cost of evaluating the flux function derivative (or Jacobian) and the cost of directly evaluating the flux function. This ratio of this cost will vary depending on the specific flux and the implementation. For the entropy conservative fluxes for the two-dimensional compressible Euler equations [52] used in the numerical experiments in Section 7.3.2, the cost of evaluating the flux Jacobian matrix is only 1.625 times more expensive than directly evaluating the flux (both the Jacobian matrix and the flux were evaluated only for a single coordinate direction).

\(^{3}\)In our implementations of the evaluation of $f(u)$ and the Jacobian $\frac{d f}{d u}$ (computed using Theorem 2.1), we pre-allocate all output vectors and matrices for efficiency. For the implementation of $\frac{d f}{d u}$, we compute the sum $(Q \circ F)\mathbf{1}$ by looping over rows of $Q$ and accumulating contributions from $Q \circ F$ column-by-column. We access entries of $Q^T$ to take advantage of the column-major storage of matrices in Julia.
Finally, we note that if the Jacobian matrix is not explicitly required, it is possible to approximate Jacobian-vector products in a matrix-free fashion by using a finite difference approximation with much lower computational cost [20]. However, the formulas in Theorem 2.1 can also be applied in a matrix-free fashion by avoiding explicit construction of the Jacobian matrix. Moreover, unlike a finite difference approximation, the matrix-free evaluation of the formulas in this work does not incur approximation errors beyond numerical roundoff.

7.2. Two-derivative time-stepping methods

Consider a general system of ODEs
\[
\frac{du}{dt} + f(u) = 0.
\]

Two-derivative explicit time-stepping methods are constructed based on the assumption that second derivatives of \(u\) in time are available [49, 53]. The resulting schemes can achieve higher order accuracy with fewer stages and function evaluations compared to standard Runge-Kutta methods.

Let \(g(u)\) denote the second derivative of \(u\) in time
\[
g(u) = \frac{d^2u}{dt^2} = \frac{d}{dt} \frac{df}{du} = -\frac{\partial^2 f}{\partial u^2} f(u),
\]
where we have used the chain rule in the final step. The simplest two-derivative Runge-Kutta method is the one-stage second order scheme [49]
\[
u^{k+1} = u^k - \Delta t f(u^k) + \frac{\Delta t^2}{2} g(u^k),
\]
where \(u^k\) denotes the solution at the \(k\)th time-step. We examine the one-stage, two-stage, and three-stage two-derivative Runge Kutta given in [49], which we refer to as TDRK-1, TDRK-2, TDRK-3. These schemes are second, fourth, and fifth order accurate, respectively. We also provide reference results using a low-storage 4th order 5-stage Runge-Kutta method (RK-45).

We examine the performance of two-derivative time-stepping methods for the one-dimensional Burgers’ and shallow water equations using an entropy conservative and entropy stable spectral (Lobatto) collocation method of degree \(N = 40\) on a single periodic domain \([-1, 1]\). For the entropy stable scheme, we apply a local Lax-Friedrichs penalty at the boundaries to produce entropy dissipation. We compute \(L^2\) errors for a manufactured solution, with all solution components have the form \(\sin(kt) \sin(\pi x)\) with \(k = 100\). Because TDRK methods require both first and second time derivative information, we include both source terms \(f(x,t)\) and time derivatives of source terms \(\frac{\partial f}{\partial t}\) which are computed from the manufactured solution.

Figure 2 plots \(L^2\) errors (computed using a higher accuracy Gaussian quadrature rule at final time \(T = 5\)) against the time-step size, while Table 2 shows computed rates of convergence for each TDRK scheme. We observe that all except one TDRK scheme achieves the expected rate of convergence up until the point at which errors are affected by numerical roundoff. The outlier is the TDRK-3 scheme, which converges at the expected rate of \(O(\Delta t^3)\) for the shallow water equations, but achieves a higher \(O(\Delta t^6)\) rate of convergence for the Burgers’ equation. We also observe that the 4th order RK-45 scheme is slightly more accurate than the 4th order TDRK-2 scheme. As noted in [49], the 2-stage TDRK-2 scheme requires only one evaluation of \(f(u)\) and two evaluations of \(g(u)\). However, when \(g(u)\) is computed using a Jacobian-vector product, this corresponds to two evaluations of \(f(u)\) and two Jacobian-vector products. Because evaluating Jacobian-vector products are at least as expensive as evaluating \(f(u)\), it is not clear that the TDRK-2 scheme would be more efficient than either RK-45 or the standard 4-stage 4th order Runge-Kutta method in practice.

Finally, we plot the integrated entropy \(S(t) = \int_S S(u) \, dx\) over time in Figure 3. For Burgers’ equation, we do not observe significant differences in the entropy dissipation for TDRK-2 and RK-45 schemes. For

\footnote{Five different three-stage schemes are presented in [49]. We use the scheme corresponding to free parameter \(c_3 = 2/3\), which the authors report as the best performing three-stage scheme.}
Figure 2: $L^2$ errors for manufactured solutions of the Burgers and shallow water equations for three TDRK schemes under various time-step sizes. Errors for RK-45 are also included for reference.

| dt/dt₀       | 1/2 | 1/4 | 1/8 | 1/16 |
|--------------|-----|-----|-----|------|
| TDRK-1       | 1.997 | 1.999 | 2.000 | 2.000 |
| TDRK-2       | 3.999 | 4.000 | 4.000 | 4.000 |
| TDRK-3       | 6.006 | 5.993 | 5.916 | 4.842 |

(a) Burgers equation

| dt/dt₀       | 1/2 | 1/4 | 1/8 | 1/16 |
|--------------|-----|-----|-----|------|
| TDRK-1       | 2.620 | 2.003 | 2.001 | 2.001 |
| TDRK-2       | 4.002 | 4.001 | 4.001 | 4.000 |
| TDRK-3       | 4.998 | 3.757 | -2.193 |       |

(b) Shallow water equation

Table 2: Computed rates of convergence with respect to dt for different TDRK schemes (dt₀ denotes the initial time-step). Italicized numbers denote rates which are likely affected by numerical roundoff.

Figure 3: Evolution of entropy over time for TDRK-2 and RK-45 schemes using both entropy conservative (EC) and entropy stable (ES) spectral collocation formulations of the Burgers’ and shallow water equations.
the entropy conservative formulation of the shallow water equations, the TDRK-2 scheme produces slightly more entropy dissipation than RK-45; however, both two schemes produce similar entropy dissipation for the entropy stable formulation.

7.3. Time-implicit discretizations on triangular meshes

Jacobian matrices also appear in time-implicit discretizations of nonlinear ODEs. Consider the implicit midpoint rule

\[ u^{k+1} = u^k - \Delta t f \left( \frac{u^{k+1} + u^k}{2} \right). \]

This can be rewritten in the following form where \( u^{k+1/2} = \frac{u^{k+1} + u^k}{2} \)

\[ u^{k+1/2} = u^k - \frac{\Delta t}{2} f \left( u^{k+1/2} \right) \]
\[ u^{k+1} = 2u^{k+1/2} - u^k. \]

Solving for \( u^{k+1/2} \) is a nonlinear equation and can be done via Newton’s method

\[ u^{k+1/2},\ell+1 = u^{k+1/2},\ell - \left( I + \frac{\Delta t}{2} \frac{\partial f}{\partial u} \bigg|_{u^{k+1/2},\ell} \right)^{-1} \left( u^{k+1/2},\ell + \frac{\Delta t}{2} f \left( u^{k+1/2},\ell \right) - u^k \right). \]

We utilize a relative tolerance of \( 1e-11 \) for the Newton iteration, and determine the time-step \( \Delta t \) using the following estimate

\[ \Delta t = CFL \times \frac{h_{\text{min}}}{C_N}, \quad C_N = \frac{(N + 1)(N + 2)}{2}, \]

where CFL is the CFL constant, \( h_{\text{min}} \) is the size of the smallest element in the mesh, and \( C_N \) is the \( N \)-dependent trace constant for a degree \( N \) polynomial space on the reference triangle [54].5

7.3.1. 2D Burgers’ equation

We consider energy conservative and energy stable discretizations of 2D Burgers’ equation

\[ \frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial u^2}{\partial x} = 0 \]

with periodic boundary conditions on the domain \([-1,1]^2\). For the initial condition \( u(x,0) = -\sin(\pi x) \), the solution forms a shock around \( T = 1/2 \).

We discretize the Burgers’ equation using an energy conservative (or stable) scheme in space [12, 35] and an implicit midpoint discretization in time. The spatial discretization utilizes a degree \( N \) polynomial space, degree 2\( N \) volume quadrature, and an \((N+1)\)-point Gauss quadrature for faces. An energy stable scheme is constructed by adding a local Lax-Friedrichs penalization term, \(-\frac{\lambda}{2} [u]_i\), to the energy conservative flux contribution, where \( \lambda = \max (|u^+|, |u^-|) \) is the maximum wavespeed at an interface. We utilize both uniform and “squeezed” triangular meshes with very small elements (see Figure 4), the latter of which is constructed by replacing the \( x \)-coordinate \( x_i \) of each vertex with \( x_i - 3 \sin(\pi x_i) \).

Since the implicit midpoint rule is a symplectic integrator, we expect energy to be conserved up to machine precision for an energy conservative scheme. We set the initial condition randomly, remove the Lax-Friedrichs penalization, and run until time \( T = 1 \) using a CFL of 10 on both uniform and squeezed \( 8 \times 8 \) meshes with \( N = 2 \). For the uniform mesh, the total change in energy was \(-2.665e-15\). The squeezed mesh behaved similarly, with a total change in energy of \( 3.553e-15 \).

Next, we add local Lax-Friedrichs dissipation and run with the initial condition \(-\sin(\pi x)\) until time \( T = 1 \) using a CFL of 250. Figure 4 shows solutions for both cases. In each case, oscillations appear in a

---

5Trace constants \( C_N \) for other element types are derived in [55].
Figure 4: $N = 2$ solutions of Burgers’ equation at $T = 1$ on uniform and anisotropic “squeezed” $16 \times 16$ meshes.
one-element vicinity around the shock. For both meshes, the Newton iteration converges in between 4 and 7 iterations. We note that for an entropy conservative scheme with a randomly generated initial condition, increasing the CFL further resulted in non-convergence of the Newton iteration. However, either switching to the initial condition \( u(x, y, 0) = -\sin(\pi x) \) or adding local Lax-Friedrichs dissipation avoids stalling of the Newton iteration.

### 7.3.2. 2D compressible Euler equations

Finally, we consider a time-implicit discretization of the 2D compressible Euler equations

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x_1} + \frac{\partial (\rho v)}{\partial x_2} = 0,
\]

\[
\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x_1} + \frac{\partial (\rho uv)}{\partial x_2} = 0,
\]

\[
\frac{\partial \rho v}{\partial t} + \frac{\partial (\rho uv)}{\partial x_1} + \frac{\partial (\rho v^2 + p)}{\partial x_2} = 0,
\]

\[
\frac{\partial E}{\partial t} + \frac{\partial (u(E + p))}{\partial x_1} + \frac{\partial (v(E + p))}{\partial x_2} = 0,
\]

Here, \( \gamma = 1.4 \), and \( p = (\gamma - 1)\rho e \) is the pressure, where \( \rho e = E - \frac{1}{2} \rho (u^2 + v^2) \) is the specific internal energy. We construct a scheme which is stable with respect to the unique entropy for the compressible Navier-Stokes equations [5]

\[
S(u) = -\frac{\rho s}{\gamma - 1}, \quad u = [\rho, \rho u, \rho v, E]^T,
\]

where \( s = \log \left( \frac{p}{\rho} \right) \) denotes the specific entropy. Mappings between conservative variables \( u \) and entropy variables \( v = \{v_1, v_2, v_3, v_4\} \) in two dimensions are given by

\[
v_1 = \frac{\rho e(\gamma + 1 - s) - E}{\rho e}, \quad v_2 = \frac{\rho u}{\rho e}, \quad v_3 = \frac{\rho v}{\rho e}, \quad v_4 = -\frac{\rho}{\rho e},
\]

\[
\rho = -(\rho e)v_4, \quad \rho u = (\rho e)v_2, \quad \rho v = (\rho e)v_3, \quad E = (\rho e) \left( 1 - \frac{v_2^2 + v_3^2}{2v_4} \right),
\]

where \( \rho e \) and \( s \) can be expressed in terms of the entropy variables as

\[
\rho e = \left( \frac{(\gamma - 1)}{(-v_4)^{\gamma - 1}} \right)^{1/(\gamma - 1)} e^{\frac{s - \gamma}{\gamma - 1}}, \quad s = \gamma - v_1 + \frac{v_2^2 + v_3^2}{2v_4}.
\]

We utilize the entropy conservative and kinetic energy preserving finite volume fluxes derived in [52], and apply entropy dissipation by adding a local Lax-Friedrichs penalization term, \( -\lambda \frac{1}{2} ||u|| \) [6, 37]. We compute at each point on an interface the local wavespeed \( a = |u \cdot n| + c \), where \( c = \sqrt{\gamma \rho / p} \) is the sound speed and \( u \cdot n \) is the normal velocity. The local Lax-Friedrichs parameter is then computed via \( \lambda = \sqrt{(a^+ + a^-)^2 / 2} \), where \( a^+, a^- \) are computed using the interior and exterior solution states, respectively.

We employ an entropy stable modal DG formulation from [37] on triangles using total degree \( N \) polynomials. The surface quadrature is constructed using 1D \((N + 1)\) point Gauss quadrature rules on each face and we use a volume quadrature [56] which is exact for degree \( 2N \) polynomials. Since this is a non-collocated formulation, we need the change of variables matrices \( \frac{\partial u}{\partial v}, \frac{\partial v}{\partial u} \) to evaluate (19). These matrices
can be computed using automatic differentiation or using the explicit formulas [57].

\[
\begin{align*}
\frac{\partial u}{\partial v} &= \begin{bmatrix} \rho & \rho u & \rho v & E \\ \rho u & \rho u^2 + p & \rho uv & \rho uH \\ \rho v & \rho uv & \rho v^2 + p & \rho vH \\ E & \rho uH & \rho vH & \rho H^2 - c^2 \frac{p}{\gamma-1} \end{bmatrix}, \\
\frac{\partial v}{\partial u} &= -\frac{1}{\rho v^4} \begin{bmatrix} \gamma + k^2 & k v_2 & k v_3 & (k+1) v_4 \\ k v_2 & v_2^2 - v_4 & v_2 v_3 & v_2 v_4 \\ k v_3 & v_2 v_3 & v_3^2 - v_4 & v_3 v_4 \\ (k+1) v_4 & v_2 v_4 & v_3 v_4 & v_4^2 \end{bmatrix},
\end{align*}
\]

where \(c\) is the sound speed, \(H = c^2/(\gamma - 1) + \frac{1}{2}(u^2 + v^2)\) is the enthalpy, and \(k = \frac{1}{2}(v_2^2 + v_3^2)/v_4\).

There exist several choices for entropy conservative fluxes [24, 58, 52]. We utilize the the entropy conservative numerical fluxes given by Chandrashekar in [52]

\[
\begin{align*}
f^{1}_{LS}(u_L, u_R) &= \{\{\rho\}\} \log \{\{u\}\}, \\
f^{1}_{LS}(u_L, u_R) &= f^{1}_{LS} \{\{u\}\} + p_{avg}, \\
f^{2}_{LS}(u_L, u_R) &= f^{2}_{LS} \{\{u\}\}, \\
f^{2}_{LS}(u_L, u_R) &= f^{2}_{LS} \{\{v\}\} + p_{avg}, \\
f^{4}_{LS}(u_L, u_R) &= (E_{avg} + p_{avg}) \{\{u\}\}, \\
f^{4}_{LS}(u_L, u_R) &= (E_{avg} + p_{avg}) \{\{v\}\},
\end{align*}
\]

where the quantities \(p_{avg}, E_{avg}, \|u\|^2_{avg}\) are defined as

\[
\begin{align*}
p_{avg} &= \frac{\{\{\rho\}\}}{2 \{\{\beta\}\}}, \\
E_{avg} &= \frac{\{\{\rho\}\} \log \{\{\beta\}\}}{2 \{\{\beta\}\} \log (\gamma - 1)} + \frac{\|u\|^2_{avg}}{2}, \\
\|u\|^2_{avg} &= 2(\{\{u\}\}^2 + \{\{v\}\}^2) - (\{\{u^2\}\} + \{\{v^2\}\}) = u^+ u + v^+ v,
\end{align*}
\]

where \(\{\{u\}\} = \frac{1}{2} (u^+ + u)\), where \(u^+, u\) denotes the exterior and interior states across the interface of an element \(D^k\).

Let \(S(t) = \int_\Omega S(u(x,t))\) denote the total entropy in the domain \(\Omega\), where the integral is approximated using the same quadrature rule used to construct the DG mass matrix over each element. We begin by checking the change in entropy \(S(t) - S(0)\) for an entropy conservative formulation. We utilize a discontinuous initial condition

\[\rho = \begin{cases} 1.1 & -0.5 \leq x, y \leq 0.5, \\
1 & \text{otherwise}, \quad u, v = 0, \quad E = \rho^\gamma. \end{cases}\]

A triangular mesh is constructed by bisecting each element in a uniform mesh of \(8 \times 8\) quadrilaterals, and the solution is evolved until final time \(T = 10\). Figure 5 shows the results for \(N = 2\) and \(N = 3\) for \(\text{CFL} = \frac{1}{4}\) and \(\text{CFL} = \frac{1}{8}\). We observe that halving the CFL reduces the change in entropy by a factor of 4, which corresponds to the second order time accuracy of the implicit midpoint rule. We also check the entropy dissipation for different CFL numbers in Figure 6. Both \(N = 2\) and \(N = 3\) display similar results, with dissipation decreasing as the CFL increases. We also note that the number of Newton iterations remains relatively constant for different time-step sizes: for \(\text{CFL} = .1\), Newton converged in 3 – 4 iterations, for \(\text{CFL} = 1\), Newton converged in 4 – 5 iterations, and for \(\text{CFL} = 10\), Newton converged in 5 – 6 iterations. We also tried \(\text{CFL} = 100\) over a longer time period, for which Newton also converged in 5 – 6 iterations. However, for initial conditions with sufficiently large variations, Newton did not converge for \(\text{CFL} = 100\).

Finally, we examine the behavior of the implicit midpoint method with respect to variations in element size. We use the isentropic vortex analytic solution (centered at \(x = 0, y = 5\)) on the domain \([-5, 5] \times [0, 20]\). We compute the \(L^2\) error at time \(T = 5\) for a uniform and “squeezed” anisotropic triangular mesh, both of which are constructed by bisecting each element of a uniform \(24 \times 16\) quadrilateral mesh. Both cases use a degree \(N = 3\) approximation and time-step of \(dt = .1\), and Figure 7 shows both DG solutions with the
Figure 5: Change in entropy over time for entropy conservative formulations of the compressible Euler equations and the implicit midpoint method.

Figure 6: Change in entropy over time for entropy stable formulations of the compressible Euler equations and the implicit midpoint method.
mesh overlaid. The $L^2$ errors for the isentropic vortex are 0.0901 and 0.0935 on the uniform and “squeezed” meshes, respectively, suggesting that implicit entropy stable formulations robustly handle settings where the maximum stable time-step for explicit methods is restricted by minimum element size.

8. Conclusion

In this work, we derive efficient formulas for Jacobian matrices resulting from entropy conservative and entropy stable schemes based on flux differencing and summation-by-parts operators. Formulas for both finite difference summation-by-parts and modal DG formulations are derived and the resulting matrices are applied to both two-derivative explicit Runge Kutta methods and implicit time-stepping schemes based on high order DG formulations of the 1D Burgers’, 1D shallow water, and 2D compressible Euler equations. Future work will investigate the application of such formulas towards preconditioners and sensitivity analysis.

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