

# RELAXATION RUNGE–KUTTA METHODS: FULLY DISCRETE EXPLICIT ENTROPY-STABLE SCHEMES FOR THE COMPRESSIBLE EULER AND NAVIER–STOKES EQUATIONS\*

HENDRIK RANOCHA<sup>†</sup>, MOHAMMED SAYYARI<sup>‡</sup>, LISANDRO DALCIN<sup>‡</sup>, MATTEO PARSANI<sup>‡</sup>, AND DAVID I. KETCHESON<sup>‡</sup>

**Abstract.** The framework of inner product norm preserving relaxation Runge–Kutta methods [D. I. Ketcheson, *SIAM J. Numer. Anal.*, 57 (2019), pp. 2850–2870] is extended to general convex quantities. Conservation, dissipation, or other solution properties with respect to any convex functional are enforced by the addition of a *relaxation parameter* that multiplies the Runge–Kutta update at each step. Moreover, other desirable stability (such as strong stability preservation) and efficiency (such as low storage requirements) properties are preserved. The technique can be applied to both explicit and implicit Runge–Kutta methods and requires only a small modification to existing implementations. The computational cost at each step is the solution of one additional scalar algebraic equation for which a good initial guess is available. The effectiveness of this approach is proved analytically and demonstrated in several numerical examples, including applications to high order entropy-conservative and entropy-stable semidiscretizations on unstructured grids for the compressible Euler and Navier–Stokes equations.

**Key words.** Runge–Kutta methods, energy stability, entropy stability, monotonicity, strong stability, invariant conservation, conservation laws, fully discrete entropy stability, compressible Euler and Navier–Stokes equations

**AMS subject classifications.** 65L20, 65L06, 65M12, 76N99

**DOI.** 10.1137/19M1263480

**1. Introduction.** Consider a time-dependent ordinary differential equation (ODE)

$$(1.1) \quad \begin{aligned} \frac{d}{dt}u(t) &= f(t, u(t)), \quad t \in (0, T), \\ u(0) &= u^0, \end{aligned}$$

in a real Hilbert space  $\mathcal{H}$  with inner product  $\langle \cdot, \cdot \rangle$ , inducing the norm  $\|\cdot\|$ . Let  $\eta: \mathcal{H} \rightarrow \mathbb{R}$  denote a smooth convex function whose correct evolution in time is important in the solution of (1.1). In relevant applications  $\eta$  might represent, e.g., some form of energy or momentum; in the present work we refer to  $\eta$  as *entropy*, with a view to applications in a hyperbolic and incompletely parabolic system of partial differential equations (PDEs) such as the compressible Euler and Navier–Stokes equations. The time evolution of  $\eta$  is given by  $\frac{d}{dt}\eta(u(t)) = \langle \eta'(u(t)), f(t, u(t)) \rangle$ . Thus entropy *dissipative* systems satisfy

$$(1.2) \quad \forall u \in \mathcal{H}, t \in [0, T]: \quad \langle \eta'(u), f(t, u) \rangle \leq 0,$$

\*Submitted to the journal’s Methods and Algorithms for Scientific Computing section May 22, 2019; accepted for publication (in revised form) November 6, 2019; published electronically March 12, 2020.

<https://doi.org/10.1137/19M1263480>

**Funding:** This work was supported by the King Abdullah University of Science and Technology (KAUST).

<sup>†</sup>TU Braunschweig, Institute Computational Mathematics, Universitätsplatz 2, 38106 Braunschweig, Germany (h.ranocha@tu-bs.de).

<sup>‡</sup>King Abdullah University of Science and Technology (KAUST), Extreme Computing Research Center (ECRC), Computer Electrical and Mathematical Science and Engineering Division (CEMSE), Thuwal, 23955-6900, Saudi Arabia (mohammed.alsayyari@kaust.edu.sa, dalcinl@gmail.com, matteo.parsani@kaust.edu.sa, david.ketcheson@kaust.edu.sa).

while entropy *conservative* ones fulfill

$$(1.3) \quad \forall u \in \mathcal{H}, t \in [0, T]: \quad \langle \eta'(u), f(t, u) \rangle = 0.$$

In many applications it is important to preserve this qualitative behavior, i.e., to ensure that

$$\eta(u^{n+1}) \leq \eta(u^n)$$

for a dissipative problem or that

$$\eta(u^{n+1}) = \eta(u^0)$$

for a conservative problem. Violation of these properties can lead to solutions that are unphysical and qualitatively incorrect. Nevertheless, most numerical methods fail to guarantee these discrete properties. In the present work, we present a modification that makes any Runge–Kutta (RK) method preserve conservation or dissipativity while also retaining other important and desirable properties of the unmodified RK method.

In this work we focus on applications to entropy conservative or entropy dissipative semidiscretizations of hyperbolic conservation laws [49, 51] and the Navier–Stokes equations (incompletely parabolic). Nevertheless, the methods presented here may be useful in many other applications, including Hamiltonian systems, dispersive wave equations, and other areas where geometric numerical integration is important.

*Remark 1.1.* It is possible to generalize this setting to Banach spaces instead of Hilbert spaces. In that case, scalar products of the form  $\langle \eta', f \rangle$  should be read as the application of the bounded linear functional  $\eta'$  to  $f$ .

**1.1. Related work.** Recently, there has been some interest in nonlinear and entropy stability of numerical methods for balance laws. Several major hurdles remain on the path toward complete nonlinearity and entropy stability of numerical algorithms because most of the research has been focused on semidiscrete schemes (see, for instance, [48, 37, 12, 56, 38, 55, 17, 18]). Stability/dissipation results for fully discrete schemes have mainly been limited to semidiscretizations including certain amounts of dissipation [51, 24, 57, 40], linear equations [50, 42, 46, 47], or fully implicit time integration schemes [51, 19, 31]. For explicit methods and general equations, there are negative experimental and theoretical results concerning entropy stability [39, 32].

While applications to entropy conservative/dissipative schemes for hyperbolic and parabolic balance laws are included in this article, the general technique is not limited to this setting but can be applied to many ODEs and to both explicit and implicit RK methods. Since the basic idea is to preserve properties given at the continuous level discretely, these schemes are related to the topic of geometric numerical integration; see [22] and references therein.

The basic idea behind the methods proposed here comes from Dekker and Verwer [15, pp. 265–266] and has been developed for inner-product norms in [27]. The idea (and notation) of Dekker and Verwer [15] was applied in [16] to a restricted class of fourth order methods. This was extended in [7] by giving a general proof that applying the technique to an RK method of order  $p$  results in a method of order at least  $p - 1$ . The idea was referred to therein as the *incremental direction technique* (IDT) and viewed as an RK projection method where the search direction is the same as the direction of the next time step update. Nevertheless, the main focus in [7] is on a different type of projection in which the search direction is chosen based on

an embedded method. Grimm and Quispel [21] extended the standard orthogonal projection method [22, section IV.4] to dissipative systems possessing a Lyapunov function and the same approach was used in [8, 30] with the choice of search directions advocated in [7]. Kojima [29] reviewed some related methods and proposed another kind of projection scheme for conservative systems.

Like standard RK methods, and in contrast to orthogonal projection methods, the schemes based on the approach of Dekker and Verwer [15] or Calvo et al. [7] preserve linear invariants—a feature that is absolutely essential in the numerical solution of hyperbolic conservation laws. It is also interesting to study different projection methods since the behavior of these schemes can depend crucially on the choice of conserved quantities [22, section IV.4] and the type of projection or search direction [8, 9, 29, 34].

The goal of this article is to extend the theory developed in [27] to a much broader class of problems. The resulting schemes are shown to possess desirable properties, both theoretically and in numerical experiments. In particular, applications include fully discrete entropy stable numerical methods of any order for the three-dimensional compressible Euler and Navier–Stokes equations on unstructured grids based on summation-by-parts (SBP) operators [10, 35]. Analytical and numerical comparisons with other types of projection schemes are left for future work.

**1.2. Runge–Kutta methods.** A general (explicit or implicit) RK method with  $s$  stages can be represented by its Butcher tableau [6, 23]

$$(1.4) \quad \begin{array}{c|c} c & A \\ \hline & b^T \end{array},$$

where  $A \in \mathbb{R}^{s \times s}$  and  $b, c \in \mathbb{R}^s$ . For (1.1), a step from  $u^n \approx u(t_n)$  to  $u^{n+1} \approx u(t_{n+1})$ , where  $t_{n+1} = t_n + \Delta t$  is given by

$$(1.5a) \quad y_i = u^n + \Delta t \sum_{j=1}^s a_{ij} f(t_n + c_j \Delta t, y_j), \quad i \in \{1, \dots, s\},$$

$$(1.5b) \quad u^{n+1} = u^n + \Delta t \sum_{i=1}^s b_i f(t_n + c_i \Delta t, y_i).$$

Here,  $y_i$  are the stage values of the RK method. We will make use of the shorthand

$$(1.6) \quad f_i := f(t_n + c_i \Delta t, y_i), \quad f_0 := f(t_n, u^n).$$

As is common in the literature, we assume that  $A\mathbb{1} = c$  with  $\mathbb{1} = (1, \dots, 1)^T \in \mathbb{R}^s$ .

An RK method is (entropy) *dissipation preserving* if  $\eta(u^{n+1}) \leq \eta(u^n)$  whenever the right-hand side fulfills (1.2). Similarly, it is (entropy) *conservative* if  $\eta(u^{n+1}) = \eta(u^n)$  whenever the system satisfies (1.3). Depending on the context, such schemes are also called *monotone* or *strongly stable* [24, 39].

**2. Relaxation Runge–Kutta methods.** Following [15, pp. 265–266] and [27], the basic idea to make a given RK method entropy stable is to scale the weights  $b_i$  by a parameter  $\gamma_n \in \mathbb{R}$ , i.e., to use

$$(2.1) \quad u_\gamma^{n+1} := u^n + \gamma_n \Delta t \sum_{i=1}^s b_i f_i$$

instead of  $u^{n+1}$  in (1.5b) as the new value after one time step. If the entropy is just the energy  $\eta(u) = \frac{1}{2}\|u\|^2$ , the choice of  $\gamma_n$  proposed in [27] is such that

$$(2.2) \quad \frac{1}{2}\|u_\gamma^{n+1}\|^2 - \frac{1}{2}\|u^n\|^2 = \gamma_n \Delta t \sum_{i=1}^s b_i \langle y_i, f_i \rangle.$$

The new generalization to entropy stability proposed in this article is to enforce the condition

$$(2.3) \quad \eta(u_\gamma^{n+1}) - \eta(u^n) = \gamma_n \Delta t \sum_{i=1}^s b_i \langle \eta'(y_i), f_i \rangle$$

by finding a root  $\gamma_n$  of

$$(2.4) \quad r(\gamma) = \eta\left(u^n + \gamma \Delta t \sum_{i=1}^s b_i f_i\right) - \eta(u^n) - \gamma \Delta t \sum_{i=1}^s b_i \langle \eta'(y_i), f_i \rangle.$$

Note that the direction

$$(2.5) \quad d^n := \sum_{i=1}^s b_i f_i$$

and the estimate of the entropy change

$$(2.6) \quad e := \Delta t \sum_{i=1}^s b_i \langle \eta'(y_i), f_i \rangle$$

can be computed on the fly during the computation of the RK method and are not influenced by  $\gamma_n$ . Hence, existing low-storage implementations can be used. In the end, finding a root of  $r(\gamma) = \eta(u^n + \gamma d) - \eta(u^n) - \gamma e$  is just a scalar root finding problem for the convex function  $r$ .

*Remark 2.1.* If  $f$  is a semidiscretization of a (hyperbolic) PDE with entropy  $S$  and entropy variables  $w(u) = S'(u)$  in the domain  $\Omega$ , (2.4) corresponds to a discrete version of

$$(2.7) \quad r(\gamma) = \int_\Omega S(u^n + \gamma \Delta t d^n) \, d\Omega - \int_\Omega S(u^n) \, d\Omega - \gamma \Delta t \sum_{i=1}^s b_i \int_\Omega w_i \cdot f_i \, d\Omega,$$

since the total entropy is  $\eta(u) = \int_\Omega S(u) \, d\Omega$ .

If  $f$  is a semidiscretization of a PDE and  $\eta$  the global entropy,  $r(\gamma = 1)$  can be interpreted as global entropy production of the unmodified RK method. Indeed,  $\eta(u^{n+1}) - \eta(u^n)$  is the global entropy change and  $e$  is the entropy change, which has the same sign as the true entropy time derivative if the weights  $b_i \geq 0$ . Hence,  $r$  will sometimes be called *temporal entropy production*. Thus, finding a root of  $r$  yields a scheme that is entropy conservative for conservative problems and entropy dissipative for dissipative problems. This can be viewed as an extension of [27, Theorem 2.1], which dealt only with inner-product norms.

**THEOREM 2.2.** *The method defined by (1.5a) and (2.1), where  $\gamma_n$  is a root of (2.4), is conservative. If the weights  $b_i$  are nonnegative and  $\gamma_n \geq 0$ , then the method is dissipation preserving.*

The new numerical solution  $u_\gamma^{n+1}$  can be interpreted as an approximation to either  $u(t_n + \Delta t)$  (with scaled weights  $\gamma_n b_i$ ) or to  $u(t_n + \gamma_n \Delta t)$  (with scaled time step  $\gamma_n \Delta t$ ). As mentioned in [27], the given RK method determines the direction  $d$  and  $\gamma_n$  can be interpreted as a relaxation parameter determined by the requirement of preserving the evolution of  $\eta$ . Hence, the method defined by (1.5a) and (2.1) with the interpretation  $u_\gamma^{n+1} \approx u(t_n + \gamma_n \Delta t)$  is called a *relaxation RK* (RRK) method. The scheme using  $u_\gamma^{n+1} \approx u(t_n + \Delta t)$  will be referred to as an IDT method [7].

**Remark 2.3.** Some well-known RK schemes do not satisfy the sufficient condition  $b_i \geq 0$ ,  $i \in \{1, \dots, s\}$ . For example, the classical fifth/fourth order pairs of Fehlberg and Dormand and Prince have negative coefficients  $b_5 < 0$ .

**2.1. Existence of a solution.** RRK methods have been developed in [27] for the preservation of inner product norms; in that setting  $r(\gamma)$  is quadratic and its roots can be explicitly computed. Here we deal instead with arbitrary functionals; as we will see, new techniques are required.

Obviously,  $r(0) = 0$  and  $r$  is convex since the entropy  $\eta$  is convex. There is a positive root of  $r$  if and only if  $r(\gamma)$  is negative for small  $\gamma > 0$  and positive for large enough  $\gamma > 0$ .

**LEMMA 2.4.** *Let an RK method be given with coefficients such that  $\sum_{i=1}^s b_i a_{ij} > 0$  and let  $r(\gamma)$  be defined by (2.4). If  $\eta''(u^n)(f_0, f_0) > 0$ , then  $r'(0) < 0$  for sufficiently small  $\Delta t > 0$ .*

*Proof.* By the definition of  $r$  (2.4),

$$\begin{aligned} r'(0) &= \Delta t \sum_{i=1}^s b_i \langle \eta'(u^n), f_i \rangle - \Delta t \sum_{i=1}^s b_i \langle \eta'(y_i), f_i \rangle \\ (2.8) \quad &= -\Delta t \sum_{i=1}^s b_i \int_0^1 \eta'' \left( u^n + v \Delta t \sum_{k=1}^s a_{ik} f_k \right) \left( f_i, \Delta t \sum_{j=1}^s a_{ij} f_j \right) dv. \end{aligned}$$

Using Taylor expansions of  $f_i, f_j = f_0 + \mathcal{O}(\Delta t)$ ,

$$(2.9) \quad r'(0) = -\Delta t^2 \sum_{i,j=1}^s b_i a_{ij} \int_0^1 \eta'' \left( u^n + v \Delta t \sum_{k=1}^s a_{ik} f_k \right) (f_0, f_0) dv + \mathcal{O}(\Delta t)^3.$$

Using the given assumptions,  $r'(0) < 0$  for sufficiently small  $\Delta t > 0$ .  $\square$

**Remark 2.5.** The assumption  $\sum_{i=1}^s b_i a_{ij} > 0$  is satisfied for all (at least) second order accurate RK methods since  $\sum_{i=1}^s b_i a_{ij} = 1/2$  is a condition for second order accuracy.

**LEMMA 2.6.** *Let an RK method be given with coefficients satisfying  $\sum_{i,j=1}^s b_i (a_{ij} - b_j) < 0$ . If  $\eta''(u^n)(f_0, f_0) > 0$ , then  $r'(1) > 0$  for sufficiently small  $\Delta t > 0$ .*

*Proof.* By definition of  $r$  (2.4),  
 (2.10)

$$\begin{aligned} r'(1) &= \Delta t \sum_{i=1}^s b_i \langle \eta'(u^{n+1}), f_i \rangle - \Delta t \sum_{i=1}^s b_i \langle \eta'(y_i), f_i \rangle \\ &= -\Delta t \sum_{i=1}^s b_i \int_0^1 \eta'' \left( u^{n+1} + v \Delta t \sum_{k=1}^s (a_{ik} - b_k) f_k \right) \left( f_i, \Delta t \sum_{j=1}^s (a_{ij} - b_j) f_j \right) dv. \end{aligned}$$

Using Taylor expansions of  $f_i, f_j = f_0 + \mathcal{O}(\Delta t)$ ,  
 (2.11)

$$r'(1) = -\Delta t^2 \sum_{i,j=1}^s b_i (a_{ij} - b_j) \int_0^1 \eta'' \left( u^{n+1} + v \Delta t \sum_{k=1}^s (a_{ik} - b_k) f_k \right) (f_0, f_0) dv + \mathcal{O}(\Delta t)^3.$$

Using the given assumptions,  $r'(1) > 0$  for sufficiently small  $\Delta t > 0$ . □

*Remark 2.7.* The assumption  $\sum_{i,j=1}^s b_i (a_{ij} - b_j) < 0$  is satisfied for all (at least) second order accurate RK methods since  $\sum_{i,j=1}^s b_i (a_{ij} - b_j) = \frac{1}{2} - 1 = -\frac{1}{2}$  in that case.

Together, these results establish the existence of a positive root of  $r$ .

**THEOREM 2.8.** *Assume that the RK method satisfies  $\sum_{i=1}^s b_i a_{ij} > 0$  and  $\sum_{i,j=1}^s b_i (a_{ij} - b_j) < 0$ , which is true for all (at least) second order accurate schemes. If  $\eta''(u^n)(f_0, f_0) > 0$ ,  $r$  (2.4) has a positive root for sufficiently small  $\Delta t > 0$ .*

*Proof.* Since  $r(0) = 0$  and  $r'(0) < 0$ ,  $r(\gamma) < 0$  for small  $\gamma > 0$ . Because  $r'(1) > 0$  and  $r$  is convex,  $r'$  is monotone. Hence, there must be a positive root of  $r$ . □

*Remark 2.9.* The value  $\eta''(u^n)(f_0, f_0)$  of the quadratic form  $\eta''(u^n)$  is positive for a strictly convex entropy  $\eta$  if  $f_0 \neq 0$ . If  $f_0 = 0$  and the system is autonomous, every explicit RK method will yield a stationary solution. The results of Lemmas 2.4 and 2.6 and hence of Theorem 2.8 still hold if we instead assume only that  $\eta''(f_i, f_i) > 0$  for some intermediate stage  $i$ , since the Taylor series can be expanded around that value.

*Remark 2.10.* The proof of Theorem 2.8 reveals another property of  $r$ : the temporal entropy dissipation. Since  $r$  is convex, there are exactly two distinct roots of  $r$ , namely, zero, and the desired positive root  $\gamma_n$  (if the assumptions of Theorem 2.8 are satisfied). Additionally,  $r(\gamma) \rightarrow \infty$  for  $\gamma \rightarrow \pm\infty$ . Therefore, choosing a value of  $\gamma > 0$  smaller than the positive root of  $r$  results in some additional temporal entropy dissipation, because  $r(\gamma) < 0$  in that case.

**2.2. Accuracy.** At first glance, the method described above seems to be not even consistent, since  $\gamma_n \sum_j b_j = \gamma_n \neq 1$  in general. Nevertheless, an RRK scheme is of at least the same order of accuracy as the RK scheme it is based on. In order to prove this, we obtain several results, which will be combined and are also interesting on their own. Readers who are interested only in the statement of the main accuracy result can skip these parts and continue with Theorem 2.15 and Remark 2.16.

The following result has been obtained in [27, Theorem 2.4].

**THEOREM 2.11.** *Let the given RK method be of order  $p$ . Consider the IDT/RRK method defined by (1.5a) and (2.1) and suppose that  $\gamma_n = 1 + \mathcal{O}(\Delta t^{p-1})$ .*

1. *The IDT method interpreting  $u_\gamma^{n+1} \approx u(t_n + \Delta t)$  has order  $p - 1$ .*
2. *The relaxation method interpreting  $u_\gamma^{n+1} \approx u(t_n + \gamma_n \Delta t)$  has order  $p$ .*

Using  $u^n$  as the initial value for  $u$  at  $t_n$ , an RK method with order of accuracy  $p$  yields

$$\begin{aligned}
 \eta(u^{n+1}) - \eta(u^n) &= \eta(u(t_n + \Delta t)) - \eta(u^n) + \mathcal{O}(\Delta t^{p+1}) \\
 (2.12) \quad &= \int_{t_n}^{t_n + \Delta t} \langle \eta'(u(t)), f(t, u(t)) \rangle dt + \mathcal{O}(\Delta t^{p+1}) \\
 &= \Delta t \sum_{i=1}^s b_i \langle \eta'(u(t_n + c_i \Delta t)), f(t_n + c_i \Delta t, u(t_n + c_i \Delta t)) \rangle + \mathcal{O}(\Delta t^{p+1})
 \end{aligned}$$

because of the required accuracy as a quadrature rule. Although the stage values  $y_i$  are not necessarily high order approximations of  $u(t_n + c_i \Delta t)$ , the RK order conditions guarantee

$$(2.13) \quad \sum_{i=1}^s b_i f(t_n + c_i \Delta t, y_i) = \sum_{i=1}^s b_i f(t_n + c_i \Delta t, u(t_n + c_i \Delta t)) + \mathcal{O}(\Delta t^p).$$

Hence, it is interesting to know whether  $f$  can be replaced by any smooth function in this equation.

**THEOREM 2.12.** *Let  $W$  be a Banach space,  $\psi: [0, T] \times \mathcal{H} \rightarrow W$  a smooth function, and  $b_i, c_i$  coefficients of an RK method of order  $p$ . Then*

$$(2.14) \quad \sum_{i=1}^s b_i \psi(t_n + c_i \Delta t, y_i) = \sum_{i=1}^s b_i \psi(t_n + c_i \Delta t, u(t_n + c_i \Delta t)) + \mathcal{O}(\Delta t^p).$$

**COROLLARY 2.13.** *If  $\eta$  is smooth and the given RK method is  $p$ th order accurate,  $r(\gamma = 1) = \mathcal{O}(\Delta t^{p+1})$ .*

*Proof of Corollary 2.13.* Apply Theorem 2.12 to  $\psi(t, u) = \langle \eta'(u), f(t, u) \rangle$  and use (2.12), resulting in

$$(2.15) \quad \eta(u^{n+1}) - \eta(u^n) = \Delta t \sum_{i=1}^s b_i \langle \eta'(y_i), f(t_n + c_i \Delta t, y_i) \rangle + \mathcal{O}(\Delta t^{p+1}). \quad \square$$

*Proof of Theorem 2.12.* Consider  $\phi(t) = \int_{t_n}^t \psi(\tau, u(\tau)) d\tau$ . Applying the RK method to the extended ODE (with a slight abuse of notation)

$$(2.16) \quad \underbrace{\frac{d}{dt} \begin{pmatrix} \phi(t) \\ u(t) \end{pmatrix}}_{=x(t)} = \begin{pmatrix} \psi(t, u(t)) \\ f(t, u(t)) \end{pmatrix}, \quad t \in (t_n, T), \quad \begin{pmatrix} \phi(t_n) \\ u(t_n) \end{pmatrix} = \begin{pmatrix} 0 \\ u^n \end{pmatrix},$$

yields the same stage values  $y_i$  for the second component  $u$  of  $x$ . Since the method is  $p$ th order accurate,

$$(2.17) \quad \Delta t \sum_{i=1}^s b_i \psi(t_n + c_i \Delta t, y_i) = \phi^{n+1} = \phi(t_n + \Delta t) + \mathcal{O}(\Delta t^{p+1}).$$

Additionally,  
(2.18)

$$\phi(t_n + \Delta t) = \int_{t_n}^{t_n + \Delta t} \psi(t, u(t)) dt = \Delta t \sum_{i=1}^s b_i \psi(t_n + c_i \Delta t, u(t_n + c_i \Delta t)) + \mathcal{O}(\Delta t^{p+1}).$$

Combining (2.17) and (2.18) yields the desired result.  $\square$

*Remark 2.14.* Theorem 2.12 can be seen as a superconvergence result for integrals evaluated using the quadrature rule associated with an RK method. It extends a related result of [27, Lemma 4] in two ways. First, general functionals instead of the energy are considered. Second, the proof is simplified and does not rely on extensive computations involving the theory of Butcher series.

**THEOREM 2.15.** *Assume that the conditions of Theorem 2.8 are satisfied. Hence, there exists a unique positive root  $\gamma_n$  of  $r$  (2.4). Consider the IDT/RRK method defined by (1.5a) and (2.1) and suppose that the given RK method is  $p$ th order accurate.*

1. *The IDT method interpreting  $u_{\gamma}^{n+1} \approx u(t_n + \Delta t)$  has order  $p - 1$ .*
2. *The relaxation method interpreting  $u_{\gamma}^{n+1} \approx u(t_n + \gamma_n \Delta t)$  has order  $p$ .*

*Proof.* Because of Corollary 2.13,  $r(1) = \mathcal{O}(\Delta t^{p+1})$ . As can be seen in the proof of Lemma 2.6,  $r'(1) = c\Delta t^2 + \mathcal{O}(\Delta t^3)$ , where  $c > 0$ . Hence, there is a root  $\gamma_n = 1 + \mathcal{O}(\Delta t^{p-1})$  of  $r$  (2.4). Applying Theorem 2.11 yields the desired accuracy result.  $\square$

*Remark 2.16.* As an extension of Remark 2.10, the behavior of the temporal entropy dissipation  $r$  (2.4) can be described as follows for sufficiently small  $\Delta t$  if the assumptions of Theorem 2.8 are satisfied: First,  $r(0) = 0$ ,  $r(1) = \mathcal{O}(\Delta t^{p+1}) \approx 0$ , and there is a unique  $0 < \gamma_n = 1 + \mathcal{O}(\Delta t^{p-1})$  such that  $r(\gamma_n) = 0$ . Between zero and this root of  $r$ , the values of  $r$  are negative, i.e., additional entropy dissipation is introduced in that region. Outside of the bounded interval given by zero and  $\gamma_n$ ,  $r$  is positive and the time integration scheme produces entropy. Additionally,  $r(\gamma) \rightarrow \infty$  for  $\gamma \rightarrow \pm\infty$ . Finally,  $r$  is convex and looks approximately similar to a parabola with the same roots for sufficiently small  $\Delta t > 0$ . See Figure 1(a) for a typical plot of  $r(\gamma)$ .

*Remark 2.17.* Theorem 2.15 gives a guaranteed minimal order of accuracy. For some specific problems and schemes, the resulting order of accuracy can be even greater. For example, applying the classical third order, three stage method of Heun to the harmonic oscillator

$$(2.19) \quad u_1'(t) = -u_2(t), \quad u_2'(t) = u_1(t),$$

with entropy (energy)  $\eta(u) = \|u\|^2/2$ , it can be shown that with relaxation the rate of convergence is *fourth order*. The same result holds true for a nonlinear oscillator given by

$$(2.20) \quad u_1'(t) = -\|u\|^2 u_2(t), \quad u_2'(t) = \|u\|^2 u_1(t),$$

and the same entropy  $\eta$ .

**2.3. Additional properties and generalizations.** As described in [27], relaxation RK methods still conserve linear invariants, although  $\gamma_n$  is determined in a nonlinear way. Such linear invariants are, e.g., the total mass for a semidiscretization of a hyperbolic conservation law in a periodic domain.

Another desirable stability property of numerical time integration schemes is the preservation of convex stability properties that hold for the explicit Euler method. Such schemes are called *strong stability preserving* (SSP), as described in the monograph [20] and references cited therein. It has been shown in [27, section 3] that the relaxation modification of many SSP methods retains the same SSP property of the original method as long as  $\gamma_n$  deviates not too much from unity.

If there are several convex quantities  $\eta_i$  which do not necessarily have to be conserved but might also be dissipated, one could compute a relaxation factor  $\gamma_{n,i}$  for every  $\eta_i$  and choose  $\gamma_n = \min_i \gamma_{n,i}$ . The resulting scheme will dissipate every entropy (if  $b_i \geq 0$ ) because of the general shape of the temporal entropy dissipation  $r$  (cf. Remark 2.16).

If concave quantities (which shall typically increase) are of interest, they can be treated in the same framework using a sign change of  $\eta$ . If general functions  $\eta$  without any convexity/concavity assumptions are of interest, relaxation and IDT methods can still be applied.

**PROPOSITION 2.18.** *Suppose that the given RK method is  $p$ th order accurate with  $p \geq 2$ . If  $\langle \eta'(u^{n+1}), d^n / \|d^n\| \rangle = B(u^n)\Delta t + \mathcal{O}(\Delta t^2)$  with  $B(u^n) \neq 0$ , then  $r$  (2.4) has a positive root  $\gamma_n = 1 + \mathcal{O}(\Delta t^{p-1})$ . If this root is used to define IDT/RRK methods by (1.5a) and (2.1), then the following hold:*

1. *The IDT method interpreting  $u_\gamma^{n+1} \approx u(t_n + \Delta t)$  has order  $p - 1$ .*
2. *The relaxation method interpreting  $u_\gamma^{n+1} \approx u(t_n + \gamma_n \Delta t)$  has order  $p$ .*

*Proof.* The proof of [8, Theorem 2] using the implicit function theorem can be adapted to this setting; the normalized search direction considered there is  $w = d^n / \|d^n\|$  and the projected value is  $u_\gamma^{n+1} = u^{n+1} + (1 - \gamma_n)\Delta t d^n = u^{n+1} + \lambda_n w$ , i.e., the step parameters are related via  $\gamma_n = 1 + \lambda_n / \|\Delta t d^n\|$ . Since there is a solution  $\lambda_n = \mathcal{O}(\Delta t^p)$  and  $\Delta t d^n = \Delta t \sum_{i=1}^s b_i f_i$  scales as  $\Delta t$ , there is a solution  $\gamma_n = 1 + \mathcal{O}(\Delta t^{p-1})$ . Applying Theorem 2.11 yields the desired results.  $\square$

*Remark 2.19.* While Proposition 2.18 can be applied to general functions  $\eta$ , the detailed existence and accuracy results developed in the previous sections reveal more properties in the convex case and provide additional insights. These additional properties (such as the general shape of  $r$ , possible entropy dissipation by smaller values of  $\gamma_n$ ) are useful for applications and root finding procedures.

**2.4. Implementation.** For a given RK method with coefficients  $a_{ij}$ ,  $b_i$ , the relaxation method defined by (1.5a) and (2.1) requires additionally only the solution of a scalar equation, which can be done effectively using standard methods. The derivative of  $r$  is

$$(2.21) \quad r'(\gamma) = \langle \eta'(u^n + \gamma \Delta t d^n), \Delta t d^n \rangle - e,$$

where the direction  $\Delta t d^n$  and the estimate  $e$  are defined as in (2.4) and (2.6), respectively.

For most of the numerical experiments presented below, `scipy.optimize.brentq` (using Brent's method [5, Chapters 3–4]) or `scipy.optimize.root` with `method='lm'` (using a modification of the Levenberg–Marquardt algorithm as implemented in MINPACK [33]) from SciPy [25] have been used. In most cases, Brent's method is more efficient. For the first step,  $\gamma = 1$  is a good initial guess; cf. section 2.2. In subsequent steps the previous value of  $\gamma$  is chosen as the initial guess, since  $\gamma$  changes only slightly from step to step. Implementations used for the numerical examples up to section 3.4 are provided in [41].

In particular for any convex entropy  $\eta$ , standard results of numerical analysis guarantee that Newton’s method converges if the conditions of the existence and accuracy theorems are satisfied [45, Theorem 1.9]. Optimized implementations that are robust and efficient for both small (ODE) and large (PDE) problems are left for future research.

**3. Numerical examples.** The following RK methods with weights  $b_i \geq 0$  will be used in the numerical experiments. The value of  $\Delta t$  is fixed in each test and embedded error estimators are not used.

- SSPRK(2,2): Two stage, second order SSP method of [43].
- SSPRK(3,3): Three stage, third order SSP method of [43].
- SSPRK(10,4): Ten stage, fourth order SSP method of [26].
- RK(4,4): Classical four stage, fourth order method.
- BSRK(8,5): Eight stage, fifth order method of [4].
- VRK(9,6): Nine stage, sixth order method of the family developed in [54].<sup>1</sup>
- VRK(13,8): Thirteen stage, eighth order method of the family developed in [54].<sup>2</sup>

**3.1. Conserved exponential entropy.** Consider the system

$$(3.1) \quad \frac{d}{dt} \begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} = \begin{pmatrix} -\exp(u_2(t)) \\ \exp(u_1(t)) \end{pmatrix}, \quad u^0 = \begin{pmatrix} 1 \\ 0.5 \end{pmatrix},$$

with exponential entropy

$$(3.2) \quad \eta(u) = \exp(u_1) + \exp(u_2), \quad \eta'(u) = \begin{pmatrix} \exp(u_1) \\ \exp(u_2) \end{pmatrix},$$

which is conserved for the analytical solution

$$(3.3) \quad u(t) = \left( \log \left( \frac{e^{(\sqrt{e}+e)t}(\sqrt{e} + e)}{\sqrt{e} + e^{(\sqrt{e}+e)t}} \right), \log(e + e^{3/2}) - \log(\sqrt{e} + e^{(\sqrt{e}+e)t}) \right)^T.$$

The shape of  $r(\gamma)$  for the first time step using SSPRK(3,3) is shown in Figure 1(a). In accordance with the description given in Remark 2.16,  $r(0) = 0$ ,  $r(1) \approx 0$ ,  $r$  is negative between its roots and positive outside of this interval. The order of accuracy  $r(1) = \mathcal{O}(\Delta t^{p+1})$  guaranteed by Corollary 2.13 is obtained for the methods shown in Figure 1(b).

Results of a convergence study in this setup are shown in Figure 1(a). The unmodified and relaxation schemes ( $u_\gamma^{n+1} \approx u(t^n + \gamma_n \Delta t)$ ) converge with the expected order of accuracy  $p$ , in accordance with Theorem 2.15. The IDT methods ( $u_\gamma^{n+1} \approx u(t^n + \Delta t)$ ) yield a reduced order of convergence according to Theorem 2.15. Moreover, they are far more sensitive to variations of the nonlinear solvers (algorithms, tolerances, and other related parameters) and show serious convergence issues for small time steps in this case, as can be seen in Figure 2(c). Hence, the relaxation schemes are far superior in this case.

<sup>1</sup>The coefficients are taken from <http://people.math.sfu.ca/~jverner/RKV65.IIIXb.Robust.00010102836.081204.CoeffsOnlyFLOAT> at 2019-04-27.

<sup>2</sup>The coefficients are taken from <http://people.math.sfu.ca/~jverner/RKV87.IIa.Robust.00000754677.081208.CoeffsOnlyFLOAT> at 2019-04-27.

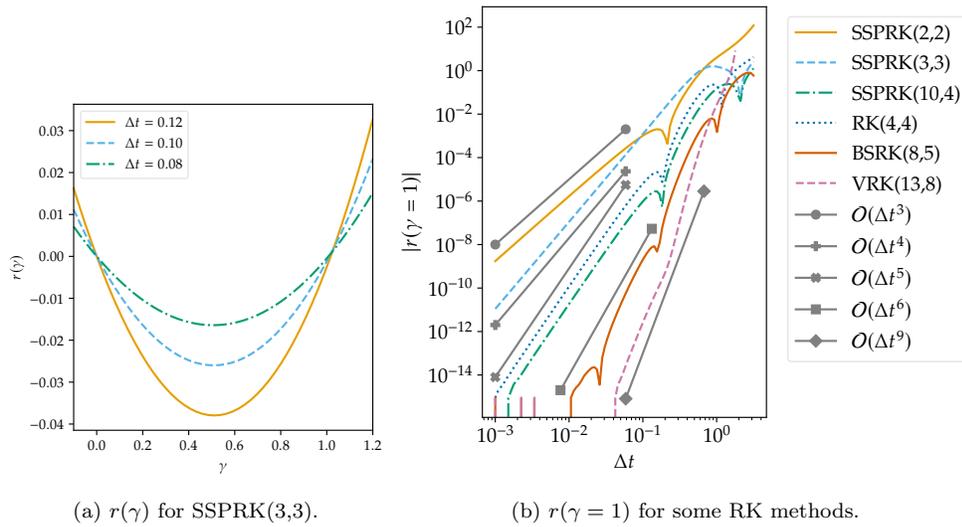


FIG. 1. Numerical results for the temporal entropy production  $r$  (2.4) at the first time step for the entropy conservative ODE (3.1).

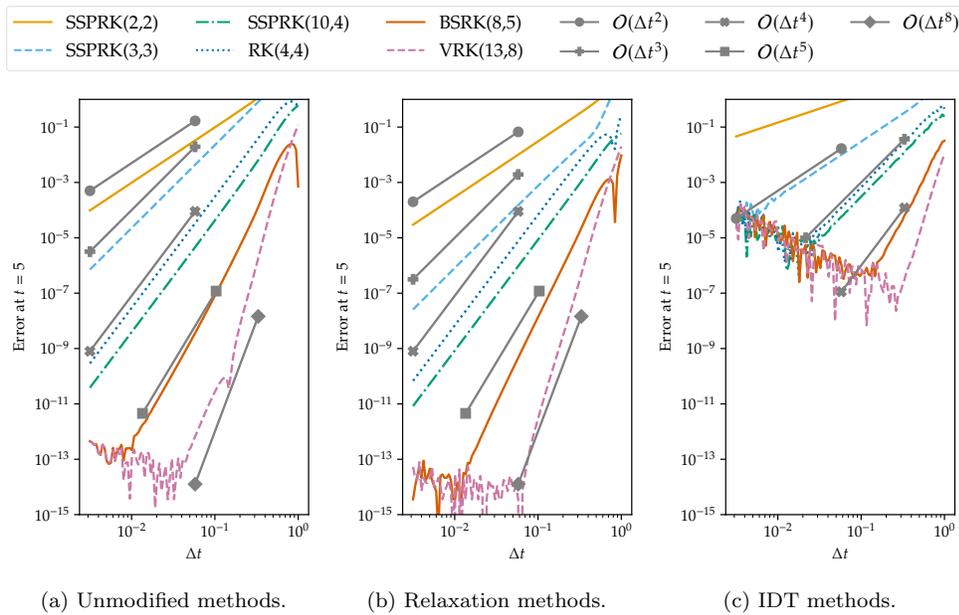


FIG. 2. Convergence study for the entropy conservative ODE (3.1) with unmodified methods, RRK schemes ( $u_\gamma^{n+1} \approx u(t^n + \gamma_n \Delta t)$ ), and IDT methods ( $u_\gamma^{n+1} \approx u(t^n + \Delta t)$ ).

**3.2. Dissipated exponential entropy.** Consider the ODE

$$(3.4) \quad \frac{d}{dt} u(t) = -\exp(u(t)), \quad u^0 = 0.5,$$

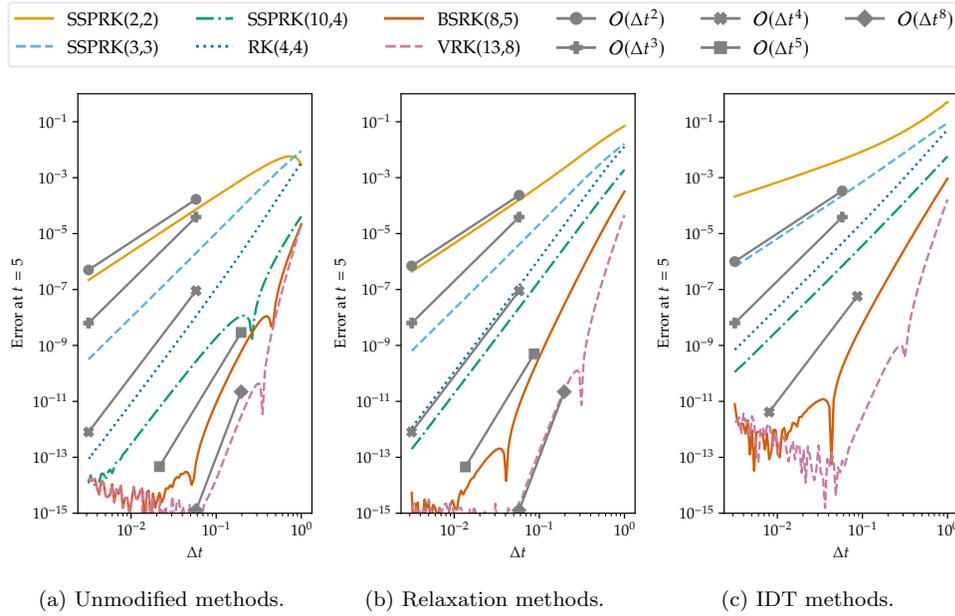


FIG. 3. Convergence study for the entropy dissipative ODE (3.4) with unmodified methods, RRK schemes ( $u_\gamma^{n+1} \approx u(t^n + \gamma_n \Delta t)$ ), and IDT methods ( $u_\gamma^{n+1} \approx u(t^n + \Delta t)$ ).

with exponential entropy  $\eta(u) = \exp(u)$ , which is dissipated for the analytical solution

$$(3.5) \quad u(t) = -\log\left(e^{-1/2} + t\right).$$

The shape of  $r$  and the convergence behavior of  $r(1) \rightarrow 0$  as  $\Delta t \rightarrow 0$  are very similar to the ones of section 3.1 and are therefore not shown in detail. However, the dissipative system (3.4) results in a better convergence behavior of the modified schemes: They depend less on the nonlinear solvers and there are fewer problems for small  $\Delta t$ , cf. Figure 3. Nevertheless, the order of convergence using the RRK schemes is still better than for the IDT methods, as explained by Theorem 2.15.

**3.3. Nonlinear pendulum.** Consider the system

$$(3.6) \quad \frac{d}{dt} \begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} = \begin{pmatrix} -\sin(u_2(t)) \\ u_1(t) \end{pmatrix}, \quad u^0 = \begin{pmatrix} 1.5 \\ 1 \end{pmatrix},$$

with nonquadratic energy

$$(3.7) \quad \eta(u) = \frac{1}{2}u_1^2 - \cos(u_2), \quad \eta'(u) = \begin{pmatrix} u_1 \\ \sin(u_2) \end{pmatrix},$$

which is conserved for all  $u$ . Further, this entropy is convex for all  $u_1$  and  $|u_2| < \frac{\pi}{2}$ . Note that the border of the convex region is crossed for this initial condition, since  $|u_2|$  becomes larger than  $\frac{\pi}{2}$ .

The energy of numerical solutions of (3.6) with  $\Delta t = 0.9$  is shown in Figure 4. As can be seen there, the energy deviates significantly for all unmodified schemes while it is conserved to machine accuracy for the RRK and IDT methods, as expected.

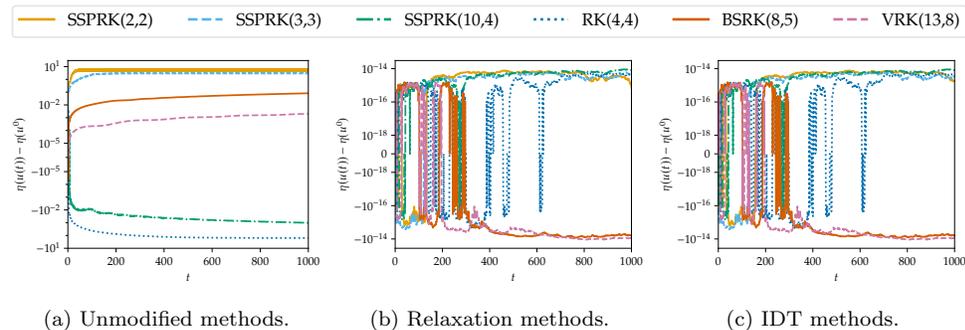


FIG. 4. Evolution of the nonquadratic energy (3.7) of numerical solutions for the nonlinear pendulum (3.6).

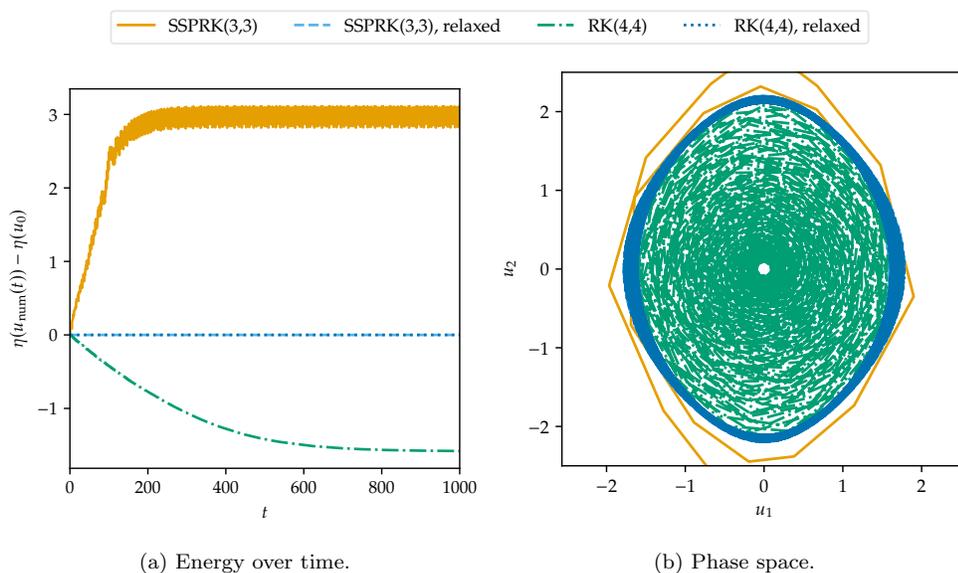


FIG. 5. Numerical solutions for the nonlinear pendulum (3.6) using the unmodified and relaxation versions of SSPRK(3,3) and RK(4,4) with  $\Delta t = 0.9$ .

Typical results for this problem are shown in Figure 5. Explicit methods tend to either create energy and drift away from the origin such as SSPRK(3,3) or to dissipate energy and drift toward the origin such as RK(4,4). In contrast, the corresponding relaxation schemes stay on the solution manifold with constant energy and show qualitatively correct long time behavior.

**3.4. Other equations.** Other systems such as the Lotka–Volterra equations with convex Lyapunov function, the harmonic oscillator with quartic entropy  $\eta(u) = \|u\|^4$ , and Burgers' equation with a logarithmic entropy have also been tested. The results are qualitatively similar to those presented above and can be found in the accompanying repository [41].

**4. The compressible Euler and Navier–Stokes equations.** In this section, we apply the relaxation time integration schemes to the compressible Euler and Navier–Stokes equations, which can be written as

$$(4.1) \quad \begin{aligned} \frac{\partial \mathcal{Q}}{\partial t} + \sum_{m=1}^3 \frac{\partial \mathcal{F}_{x_m}^{(I)}}{\partial x_m} &= \sum_{m=1}^3 \frac{\partial \mathcal{F}_{x_m}^{(V)}}{\partial x_m} & \forall (x_1, x_2, x_3) \in \Omega, \quad t \geq 0, \\ \mathcal{Q}(x_1, x_2, x_3, t) &= \mathcal{G}^{(B)}(x_1, x_2, x_3, t) & \forall (x_1, x_2, x_3) \in \Gamma, \quad t \geq 0, \\ \mathcal{Q}(x_1, x_2, x_3, 0) &= \mathcal{G}^{(0)}(x_1, x_2, x_3, 0) & \forall (x_1, x_2, x_3) \in \Omega. \end{aligned}$$

The vectors  $\mathcal{Q}$ ,  $\mathcal{F}_{x_m}^{(I)}$ , and  $\mathcal{F}_{x_m}^{(V)}$ , respectively, denote the conserved variables, the inviscid ( $I$ ) fluxes, and the viscous ( $V$ ) fluxes. The boundary data,  $\mathcal{G}^{(B)}$ , and the initial condition,  $\mathcal{G}^{(0)}$ , are assumed to be in  $L^2(\Omega)$ , with the further assumption that  $\mathcal{G}^{(B)}$  will be set to coincide with linear well-posed boundary conditions and such that entropy conservation or stability is achieved. The compressible Euler equations can be obtained from (4.1) by setting  $\mathcal{F}_{x_m}^{(V)} = 0$ .

It is well known that the compressible Navier–Stokes equations (4.1) possess a convex extension that, when integrated over the physical domain  $\Omega$ , only depends on the boundary data on  $\Gamma$ . Such an extension yields the entropy function

$$(4.2) \quad S = -\rho s,$$

where  $\rho$  and  $s$  are the density and the thermodynamic entropy, respectively. The entropy function,  $S$ , is convex with  $S'' > 0$  if the thermodynamic variables are positive and is a useful tool for proving stability in the  $L^2$  norm [13, 52].

Following the analysis described in [10, 37, 12, 17], we multiply the PDE (4.1) by the (local) entropy variables  $\mathcal{W} = \partial S / \partial \mathcal{Q}$  and arrive at the the integral form of the (scalar) entropy equation

$$(4.3) \quad \frac{d}{dt} \int_{\Omega} S d\Omega = \frac{d}{dt} \eta \leq \sum_{m=1}^3 \int_{\Gamma} \left( \mathcal{W}^{\top} \mathcal{F}_{x_m}^{(V)} - \mathcal{F}_{x_m} \right) n_{x_m} d\Gamma - DT,$$

where  $n_{x_m}$  is the  $m$ th component of the outward facing unit normal to  $\Gamma$  and

$$(4.4) \quad DT = \sum_{m,j=1}^3 \int_{\Omega} \left( \frac{\partial \mathcal{W}}{\partial x_m} \right)^{\top} \mathcal{C}_{m,j} \frac{\partial \mathcal{W}}{\partial x_j} d\Omega.$$

We remark that viscous dissipation always introduces a negative rate of change in entropy, since the  $-DT$  term in (4.3) is negative semidefinite. An increase in entropy within the domain can only result from data that convects or diffuses through the boundary  $\Gamma$ . For smooth flows, we note that the inequality sign in (4.3) becomes an equality. Finally, we highlight that the integral form of the entropy equation for the compressible Euler equations can be obtained from (4.3) by removing all the viscous terms.

Since our focus in the present work is on new time discretizations, we give only a brief explanation of the spatial discretization. We partition the physical domain  $\Omega$  with boundary  $\Gamma$  into nonoverlapping hexahedral elements and we discretize the spatial terms using a multidimensional SBP simultaneous-approximation-terms (SBP-SAT) operator as described in [10, 37, 17, 18], where the interested reader can find the details of the spatial discretization.

Using an SBP operator and its equivalent telescoping form and following closely the entropy stability analysis presented in [10, 37, 12], the total entropy of the spatial discretization satisfies

$$(4.5) \quad \frac{d}{dt} \mathbf{1}^\top \widehat{\mathbf{P}} \mathbf{S} = \frac{d}{dt} \eta = \mathbf{B}\mathbf{T} - \mathbf{D}\mathbf{T} + \Upsilon.$$

This equation mimics at the semidiscrete level each term in (4.3). Here  $\mathbf{B}\mathbf{T}$  is the discrete boundary term (i.e., the discrete version of the first integral term on the right-hand side of (4.3)),  $\mathbf{D}\mathbf{T}$  is the discrete dissipation term (i.e., the discrete version of the second term on the right-hand side of (4.3)), and  $\Upsilon$  enforces interface coupling and boundary conditions [10, 37, 12]. For completeness, we note that the matrix  $\widehat{\mathbf{P}}$  may be thought of as the mass matrix in the context of the discontinuous Galerkin finite element method.

In the next part of this section, six test cases will be considered. The first one is the propagation of an isentropic vortex for the compressible Euler equations. This test case is used to (i) perform a convergence study of the combined space and time discretizations for the compressible Euler equations and (ii) verify the entropy conservative properties of the full discretization. The second test case is the propagation of a viscous shock and is used to assess the accuracy properties of the complete entropy stable discretization for the compressible Navier–Stokes equations. The third and fourth test cases are the Sod’s shock tube and the sine-shock interaction of Titarev and Toro [53], which is the extension of the Shu–Osher problem with much more severe oscillations. These two test cases are used to show the robustness of the fully discrete entropy stable algorithm for nonsmooth solutions [10, 35]. The fifth test case is the laminar flow in a lid-driven cavity where a nonzero heat entropy flux is imposed on one of the vertical faces of the cavity. This test case is used to show the capabilities of the full discretization to capture correctly the time evolution of the entropy when, for instance, nonhomogeneous boundary conditions are imposed. Finally, the supersonic turbulent flow past a rod of square section [37] is used to demonstrate algorithmic robustness for the compressible Navier–Stokes equations.

The error is computed using the following norms:

$$(4.6) \quad \begin{aligned} \text{Discrete } L^1 : \quad & \|\mathbf{q}\|_{L^1} = \Omega_c^{-1} \sum_{j=1}^{N_{el}} \mathbf{1}^\top \mathbf{P}_j \mathbf{J}_j \text{abs}(\mathbf{q}_j), \\ \text{Discrete } L^2 : \quad & \|\mathbf{q}\|_{L^2}^2 = \Omega_c^{-1} \sum_{j=1}^{N_{el}} \mathbf{q}_j^\top \mathbf{P}_j \mathbf{J}_j \mathbf{q}_j, \\ \text{Discrete } L^\infty : \quad & \|\mathbf{q}\|_{L^\infty} = \max_{j=1 \dots N_{el}} \text{abs}(\mathbf{q}_j). \end{aligned}$$

Here  $\mathbf{J}_j$  is the metric Jacobian of the curvilinear transformation from physical space to computational space of the  $j$ th hexahedral element and  $N_{el}$  is the total number of hexahedral elements in the mesh. Furthermore,  $\Omega_c$  indicates the volume of  $\Omega$  computed as  $\Omega_c \equiv \sum_{\kappa=1}^K \mathbf{1}_\kappa^\top \widehat{\mathbf{P}}^\kappa \mathbf{J}_j \mathbf{1}_\kappa$ , where  $\mathbf{1}_\kappa$  is a vector of ones of the size of the number of nodes on the  $\kappa$ th element.

The unstructured grid solver used herein has been developed at the Extreme Computing Research Center (ECRC) at KAUST on top of the Portable and Extensible Toolkit for Scientific computing (PETSc) [2], its mesh topology abstraction (DMPLEX) [28], and scalable ODE/differential algebraic equations solver library [1].

The parameter  $\gamma_n$  of the RRK schemes is computed from (2.4) to machine precision using the bisection method which, for efficiency, is implemented directly in the unstructured grid solver.

**4.1. Propagation of an isentropic vortex in three dimensions.** In this section, we investigate the accuracy and the entropy conservation property of the full discretization obtained by combining SBP-SAT entropy conservative operators and relaxation time integration schemes. To do so, we simulate the propagation of an isentropic vortex by solving the three-dimensional compressible Euler equations. The analytical solution of this problem is

$$(4.7) \quad \begin{aligned} \mathcal{G} &= 1 - \left\{ \left[ (x_1 - x_{1,0}) - U_\infty \cos(\alpha) t \right]^2 + \left[ (x_2 - x_{2,0}) - U_\infty \sin(\alpha) t \right]^2 \right\}, \\ \rho &= T^{\frac{1}{\gamma-1}}, \quad T = \left[ 1 - \epsilon_\nu^2 M_\infty^2 \frac{\gamma-1}{8\pi^2} \exp(\mathcal{G}) \right], \\ \mathcal{U}_1 &= U_\infty \cos(\alpha) - \epsilon_\nu \frac{(x_2 - x_{2,0}) - U_\infty \sin(\alpha) t}{2\pi} \exp\left(\frac{\mathcal{G}}{2}\right), \\ \mathcal{U}_2 &= U_\infty \sin(\alpha) - \epsilon_\nu \frac{(x_1 - x_{1,0}) - U_\infty \cos(\alpha) t}{2\pi} \exp\left(\frac{\mathcal{G}}{2}\right), \quad \mathcal{U}_3 = 0, \end{aligned}$$

where  $U_\infty$  is the modulus of the free-stream velocity,  $M_\infty$  is the free-stream Mach number,  $c_\infty$  is the free-stream speed of sound, and  $(x_{1,0}, x_{2,0}, x_{3,0})$  is the vortex center. The following values are used:  $U_\infty = M_\infty c_\infty$ ,  $\epsilon_\nu = 5$ ,  $M_\infty = 0.5$ ,  $\gamma = 1.4$ ,  $\alpha = 45^\circ$ , and  $(x_{1,0}, x_{2,0}, x_{3,0}) = (0, 0, 0)$ . The computational domain is

$$x_1 \in [-5, 5], \quad x_2 \in [-5, 5], \quad x_3 \in [-5, 5], \quad t \in [0, 10].$$

The initial condition is given by (4.7) with  $t = 0$ . Periodic boundary conditions are used on all six faces of the computational domain. First, we run a convergence study for the complete entropy-stable discretization by simultaneously refining the grid spacing and the time step and keeping the ratio  $U_\infty \Delta t / \Delta x$  constant and equal to 0.05. The errors and convergence rates in the  $L^1$ ,  $L^2$ , and  $L^\infty$  norms for fourth, fifth, and sixth order accurate algorithms are reported in Table 1. We observe that the computed order of convergence in both  $L^1$  and  $L^2$  norms matches the design order of the scheme.

Next, we validate the full entropy-conservative property by simulating the propagation of the isentropic vortex using a grid with ten hexahedra in each coordinate direction and nonconforming interfaces (see Figure 6). The grid is generated by setting the solution polynomial degree in each element to a random integer chosen uniformly from the set  $\{2, 3, 4, 5\}$  [17].<sup>3</sup> All the dissipation terms used for the interface coupling [36, 17] are turned off, including upwind and interior-penalty SATs. To highlight that the space and time discretizations and their coupling are truly entropy conservative, we compute in quadruple precision.

In addition to the RK methods mentioned at the beginning of section 3, we use the following methods, which also have weights  $b_i \geq 0$ . Again, the value of  $\Delta t$  is fixed in each test, and embedded error estimators are not used.

- LSCKRK(5,4): Five stage, fourth order method of [11].
- BSRK(3,3): Three stage, third order method of [3].

<sup>3</sup>This corresponds to SBP-SAT operators which are formally third to sixth order accurate.

TABLE 1

Convergence study for the isentropic vortex using entropy conservative SBP-SAT schemes with different solution polynomial degrees  $p$  and RRK methods ( $U_\infty \Delta t / \Delta x = 0.05$ , error in the density).

$p$	RK method	$L^1$ error	$L^1$ rate	$L^2$ error	$L^2$ rate	$L^\infty$ error	$L^\infty$ rate
3	RK(4,4)	2.66E-03	—	1.36E-04	—	2.46E-02	—
		2.15E-04	3.63	1.20E-05	3.50	3.18E-03	2.95
		1.29E-05	4.06	8.50E-07	3.82	3.49E-04	3.19
		6.60E-07	4.29	5.21E-08	4.03	2.66E-05	3.71
		3.84E-08	4.10	2.82E-09	4.21	2.04E-06	3.70
4	BSRK(8,5)	3.34E-04	—	4.57E-05	—	8.50E-03	—
		3.08E-05	4.76	2.05E-06	4.48	9.06E-04	3.23
		7.33E-07	5.39	5.62E-08	5.19	5.80E-05	3.97
		2.05E-08	5.16	1.71E-09	5.04	1.33E-06	5.45
		5.70E-10	5.17	4.76E-11	5.17	3.38E-08	5.30
5	VRK(9,6)	2.23E-04	—	1.31E-05	—	3.39E-03	—
		3.55E-06	5.98	2.31E-07	5.82	8.69E-05	5.29
		6.74E-08	5.72	4.87E-09	5.57	3.25E-06	4.74
		1.10E-09	5.93	6.81E-11	6.16	7.48E-08	5.44
		1.70E-11	6.02	9.57E-13	6.15	1.64E-09	5.51

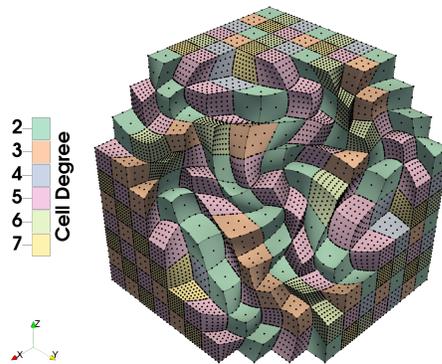


FIG. 6. Isentropic vortex: mesh cut and polynomial degree distribution with nonconforming interfaces;  $p = 2$  to  $p = 7$ .

- BSRK(7,5): Seven stage, fifth order method of [4].
- VRK(10,7): Ten stage, seventh order method of the family developed in [54].<sup>4</sup>

We show the entropy variation with and without relaxation in Figure 7. The entropy is conserved up to machine (quadruple) precision using relaxation, whereas, without relaxation, all solutions show significant changes in total entropy.

**4.2. Three-dimensional propagation of a viscous shock.** Next we study the propagation of a viscous shock using the compressible Navier–Stokes equations. We assume a planar shock propagating along the  $x_1$  coordinate direction with a Prandtl number of  $Pr = 3/4$ . The exact solution of this problem is known; the

<sup>4</sup>The coefficients are taken from <http://people.math.sfu.ca/~jverner/RKV76.IIa.Robust.000027015646.081206.CoeffsOnlyFLOAT> at 2019-05-02.

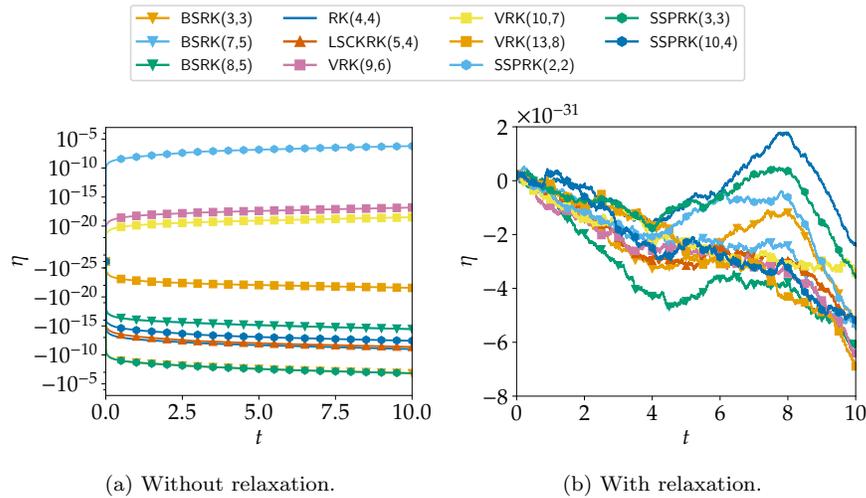


FIG. 7. *Isentropic vortex: time evolution of total entropy, using the spatial discretization shown in Figure 6.*

momentum  $\mathcal{V}(x_1)$  satisfies the ODE

$$(4.8) \quad \alpha \mathcal{V} \frac{\partial \mathcal{V}}{\partial x_1} - (\mathcal{V} - 1)(\mathcal{V} - \mathcal{V}_f) = 0, \quad -\infty \leq x_1 \leq +\infty,$$

whose solution can be written implicitly as<sup>5</sup>

$$(4.9) \quad x_1 - \frac{1}{2} \alpha \left( \log |(\mathcal{V}(x_1) - 1)(\mathcal{V}(x_1) - \mathcal{V}_f)| + \frac{1 + \mathcal{V}_f}{1 - \mathcal{V}_f} \log \left| \frac{\mathcal{V}(x_1) - 1}{\mathcal{V}(x_1) - \mathcal{V}_f} \right| \right) = 0,$$

where

$$(4.10) \quad \mathcal{V}_f \equiv \frac{\mathcal{U}_L}{\mathcal{U}_R}, \quad \alpha \equiv \frac{2\gamma}{\gamma + 1} \frac{\mu}{Pr \mathcal{M}}.$$

Here  $\mathcal{U}_{L/R}$  are known velocities to the left and right of the shock at  $-\infty$  and  $+\infty$ , respectively,  $\mathcal{M}$  is the constant mass flow across the shock,  $Pr$  is the Prandtl number, and  $\mu$  is the dynamic viscosity. The mass and total enthalpy are constant across the shock. Moreover, the momentum and energy equations become redundant.

For our tests,  $\mathcal{V}$  is computed from (4.9) to machine precision using bisection. The moving shock solution is obtained by applying a uniform translation to the above solution. The shock is located at the center of the domain at  $t = 0$  and the following values are used:  $M_\infty = 2.5$ ,  $Re_\infty = 10$ , and  $\gamma = 1.4$ . The domain is given by

$$x_1 \in [-0.5, 0.5], \quad x_2 \in [-0.5, 0.5], \quad x_3 \in [-0.5, 0.5], \quad t \in [0, 0.5].$$

The boundary conditions are prescribed by penalizing the numerical solution against the exact solution. The analytical solution is also used to furnish data for the initial conditions.

<sup>5</sup>The integration constant is taken equal to zero because the center of the viscous shock is assumed to be at  $x_1 = 0$ .

TABLE 2

Convergence study for the viscous shock using entropy stable SBP-SAT schemes with different solution polynomial degrees  $p$  and RRK methods ( $U_\infty \Delta t / \Delta x^2 = 0.05$ , error in the density).

$p$	RK method	$L^1$ error	$L^1$ rate	$L^2$ error	$L^2$ rate	$L^\infty$ error	$L^\infty$ rate
3	RK(4,4)	2.59E-02	—	3.78E-02	—	1.11E-01	—
		1.88E-03	3.79	2.81E-03	3.75	9.77E-03	3.51
		1.03E-04	4.19	1.99E-04	3.82	9.89E-04	3.30
		5.90E-06	4.13	9.97E-06	4.32	6.12E-05	4.02
		3.30E-07	4.16	5.47E-07	4.19	3.92E-06	3.97
4	BSRK(8,5)	6.80E-03	—	9.01E-03	—	2.00E-02	—
		5.74E-04	3.57	9.11E-04	3.31	4.02E-03	2.32
		2.78E-05	4.37	5.25E-05	4.12	3.32E-04	3.60
		6.30E-07	5.46	1.33E-06	5.30	1.06E-05	4.97
		1.70E-08	5.21	3.30E-08	5.33	3.59E-07	4.88
5	VRK(9,6)	3.67E-03	—	6.17E-03	—	2.53E-02	—
		1.61E-04	4.51	2.57E-04	4.59	1.24E-03	4.35
		1.34E-06	6.90	2.93E-06	6.45	2.07E-05	5.91
		1.62E-08	6.37	3.90E-08	6.23	3.94E-07	5.71

We run a convergence study for the complete entropy stable discretization by simultaneously refining the grid spacing and the time step and keeping the ratio  $U_\infty \Delta t / \Delta x^2$  constant and equal to 0.05. The errors and convergence rates in the  $L^1$ ,  $L^2$  and  $L^\infty$  norms for fourth, fifth, sixth order accurate algorithms are reported in Table 2. As for the compressible Euler equations, we observe that the order of convergence in both  $L^1$  and  $L^2$  norms is the expected one.

**4.3. Sod's shock tube.** Sod's shock tube problem is a classical Riemann problem that evaluates the behavior of a numerical method when a shock, expansion, and contact discontinuity are present. Of particular interest is smearing in the shock and contact, or oscillations at any of the discontinuities. The governing equations are the time-dependent one-dimensional compressible Euler equations which are solved in the domain given by

$$x_1 \in [0, 1], \quad t \in [0, 0.2].$$

The problem is initialized with

$$\rho = \begin{cases} 1 & x_1 < 0.5, \\ 1/8 & x_1 \geq 0.5, \end{cases} \quad p = \begin{cases} 1 & x_1 < 0.5, \\ 1/10 & x_1 \geq 0.5, \end{cases} \quad \mathcal{U}_1 = 0,$$

where  $\rho$  and  $p$  are the density and pressure, respectively. All simulations used a ratio of specific heats equal to  $7/5$ .

The entropy stable spatial discretization uses polynomials of degree  $p = 3$  and a grid with 128 elements. The problem is integrated in time using the classical fourth order accurate RK method RK(4,4).

Results of the density with and without relaxation are visually indistinguishable, as shown in Figure 8. The relaxation approach does not increase the quality of the solution and small overshoots near nonsmooth parts of the numerical approximation are visible. This behavior is expected for a spatial discretization which uses high order polynomials and no explicit shock capturing mechanism.

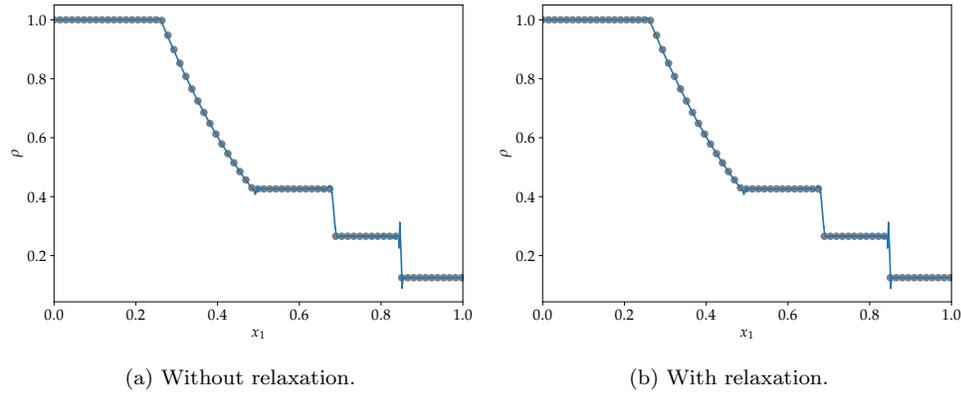


FIG. 8. Density profile of Sod's shock tube problem (exact solution shown with circles).

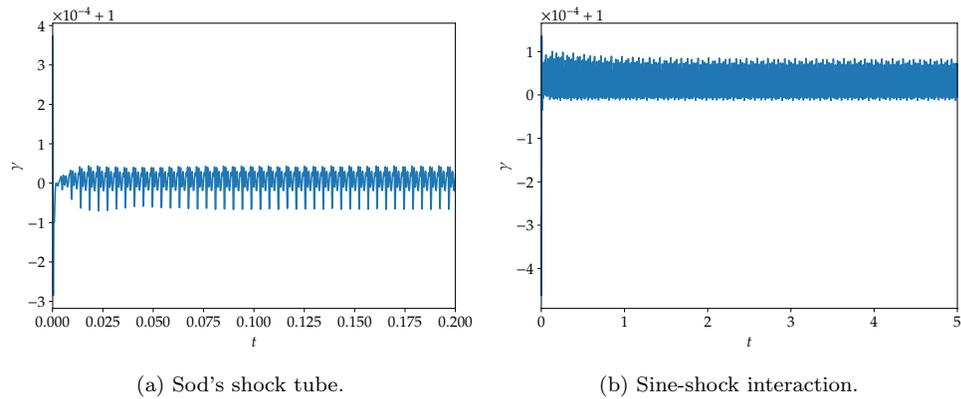


FIG. 9. Variation of the relaxation parameter,  $\gamma$ , for the shock problems.

Nevertheless, the relaxation approach does also not decrease the quality of the solution while guaranteeing the correct sign of the entropy evolution. In particular, this guarantee does not result in excessive artificial viscosity for shocks and the relaxation scheme does not smear the shock solution for a high order accurate SBP spatial scheme.

For this experiment,  $\gamma$  deviates from unity by less than  $5 \times 10^{-4}$ , as shown in Figure 9(a). After a short initial period, the value of  $\gamma$  seems to oscillate following a regular pattern with amplitude  $\lesssim 10^{-4}$ .

**4.4. Sine-shock interaction.** The solution of this benchmark problem contains both strong discontinuities and smooth structures and is well suited for testing high order shock-capturing schemes. The governing equations are the time-dependent one-dimensional compressible Euler equations which are solved in the domain given by

$$x_1 \in [-5, +5], \quad t \in [0, 5].$$

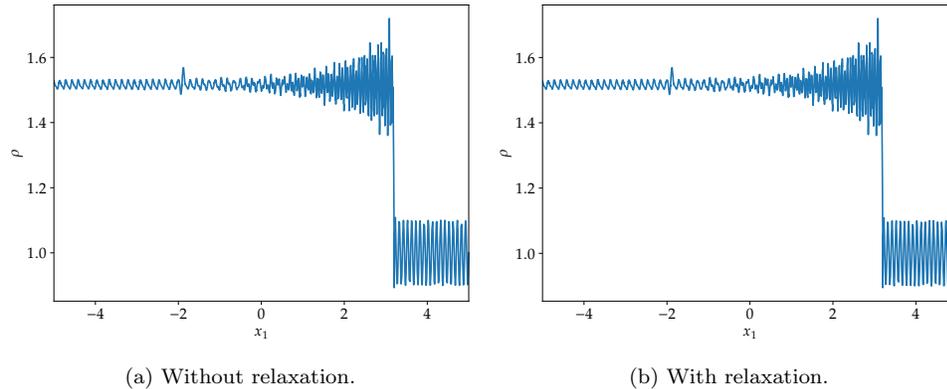


FIG. 10. Density profile of the sine-shock interaction problem.

The problem is initialized with [53]

$$(\rho, \mathcal{U}_1, p) = \begin{cases} (1.515695, 0.523346, 1.805) & \text{if } -5 \leq x < -4.5, \\ (1 + 0.1 \sin(20\pi x), 0, 1) & \text{if } -4.5 \leq x \leq 5. \end{cases}$$

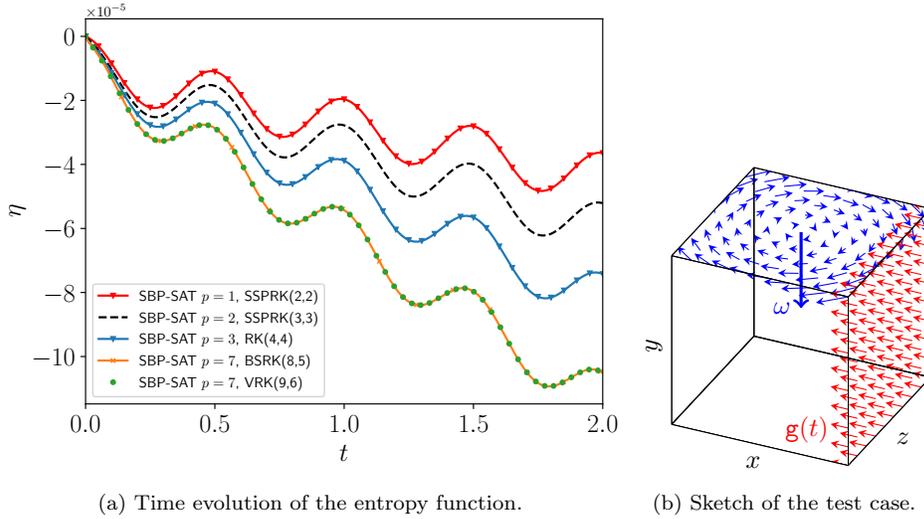
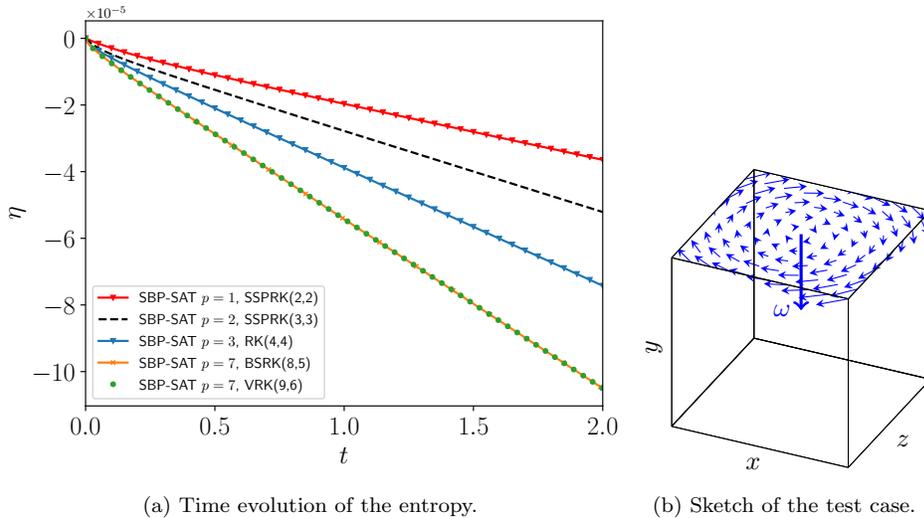
The exact solution to this problem is not available. The entropy stable semidiscretization uses polynomials of degree  $p = 3$  on a grid with 256 elements. The other parameters are the same as for Sod's shock tube problem in section 4.3.

Again, results with and without relaxation are visually indistinguishable, as shown for the density in Figure 10, supporting the conclusions of section 4.3. For this experiment,  $\gamma$  deviates from one less than  $5 \times 10^{-4}$ , as shown in Figure 9(b).

**4.5. Lid-driven cavity flow.** Next, we validate the algorithm simulating a three-dimensional lid-driven cavity flow. The domain is a cube with sides of length  $l$  discretized using a Cartesian grid composed of eight elements in each direction. A velocity field is imposed on one of the walls, corresponding to a rigid body rotation about the center of the wall at an angular speed  $\omega$  (see Figure 11(b)). We choose the rotation velocity and the size of the cavity such that this example is characterized by a Reynolds number  $Re = l^2\omega/\nu = 100$  and a Mach number  $M = l\omega/c = 0.05$ . All the dissipation terms used for the interface coupling [36] and the imposition of the boundary conditions [14] are turned off, including upwind and interior-penalty SAT terms.

First, we show the performance of some RRK schemes for the case where entropy conservative adiabatic wall boundary conditions [14] are used on all of the six faces of the cavity (see Figure 12(b)). Figure 12(a) shows the time evolution of the discrete total entropy  $\eta = \mathbf{1}^\top \widehat{\mathbf{P}} \mathbf{S}$ .

Two highly resolved numerical solutions computed with an eighth order accurate scheme ( $p = 7$ ), the BSRK(8,5), and the VRK(9,6) time integration scheme using a time adaptive algorithm with a tolerance of  $10^{-8}$  are shown in Figure 12(a). They are indistinguishable at the resolution of the plot and can be regarded as a reference solution. Because the solutions with and without relaxation are very close to each other, only the results obtained with the RRK schemes are shown. After a very short transient phase associated with the impulsive startup of the rotating plate,  $\eta$  decreases

FIG. 11. *Driven cavity with rigid body rotation  $\omega$  and nonzero heat entropy flux,  $\mathbf{g}(t)$ .*FIG. 12. *Driven cavity with rigid body rotation  $\omega$  and zero heat entropy flux.*

linearly. The reason is simple: the imposed no-slip wall boundary conditions on the six faces of the cavity are entropy conservative and the only term in (4.5) which is nonzero is  $-\mathbf{DT}$ . This contribution is strictly negative semidefinite and constant because the flow at this Reynolds number is laminar and steady, and therefore the gradient of the entropy variables in (4.4) does not change in time.

The results of three additional simulations with second, third, and fourth order accurate solvers (again with  $\Delta t = 10^{-4}$ ) are also plotted in Figure 12(a). For these methods, a fixed step size  $\Delta t = 10^{-4}$  was used. We find again that the entropy evolution with and without relaxation is indistinguishable. This demonstrates that the relaxation approach gives a stability guarantee and, unlike most numerical stabi-

lization techniques, does not (in this case) add any significant dissipation. It can be clearly seen that the rate of entropy decay is different for different entropy-conservative algorithms because of their accuracy. However, higher order discretizations give an entropy evolution that is closer to that of the the reference solution.

Next we present in Figure 11(a) the results for the same set of RRK schemes when a nonzero heat entropy flux,  $\mathbf{g}(t) = -10^{-4} \sin(4\pi t)$ , is imposed on one of the faces adjacent to the rotating face (see Figure 11(b)). Because of the added heat, the exact time evolution of the entropy is not monotonic. This can be seen in the reference solutions provided again by using an eighth order accurate spatial scheme ( $p = 7$ ) with the BSRK(8,5) and the VRK(9,6) time integration schemes using a time-adaptive algorithm with a tolerance of  $10^{-8}$ . We observe that the accuracy of the entropy evolution in time depends as expected on the order of the temporal and spatial discretizations. Again, the entropy evolution with and without relaxation is indistinguishable, indicating that the RRK methods do not add significant dissipation.

**4.6. Supersonic turbulent flow past a rod.** We finally provide further evidence of the robustness of the algorithm in the context of supersonic flow around a square cylinder with  $Re_\infty = 10^4$  and  $M_\infty = 1.5$ , which features shocks, expansion regions, and three-dimensional vortical structures [37]. The three-dimensional mesh used in the study consists of 87,872 hexahedral elements. The boundary conditions imposed are adiabatic solid wall on the square cylinder surfaces [14], periodic boundary conditions in the  $x_3$  direction, and far field at the remaining boundaries. The problem is solved using a fourth order accurate ( $p = 3$ ) spatial discretization and RK(4,4) with relaxation.

Figure 13 shows the results for the supersonic square cylinder at  $t = 130$  and the time evolution of the relaxation factor,  $\gamma$ . At  $t = 130$ , the flow is fully unsteady and the shock in front of the cylinder has reached its final position. The flow is characterized by the shock in front of the square cylinder and those in the near wake region. There is also an unsteady wake populated by three-dimensional vortices shedding from the body. The time evolution of the relaxation factor shows that the value of  $\gamma$  oscillates around one with a maximum deviation from it of  $2.5 \times 10^{-7}$ .

We finally remark that the small oscillations near the shock region are caused by discontinuities in the solution and are expected for this scheme. In fact, we are not using any shock capturing method or reducing the order of scheme at the discontinuity. Nevertheless, the simulation remains stable at all times, and the oscillations are always confined to small regions near the discontinuities. This is a feat unattainable with several alternative approaches based on linear analysis, which for this test problem lead to numerical instabilities and an almost immediate crash of the solver [37].

**5. Conclusions.** In this paper we have proposed, analyzed, and demonstrated a general approach which allows any RK method to preserve the correct time evolution of an arbitrary functional, without sacrificing linear covariance, accuracy, or stability properties of the original method. In the case of convex functionals, there are additional insights such as the possibility to add entropy dissipation by the time integration scheme. This and procedures for adaptive time step controller will be studied more deeply in the future. We are also studying the impact of relaxation on the stable time step size.

The new approach, combined with an appropriate entropy-conservative/entropy-stable semidiscretization on unstructured grids, yields the *first discretization for computational fluid dynamics* that is

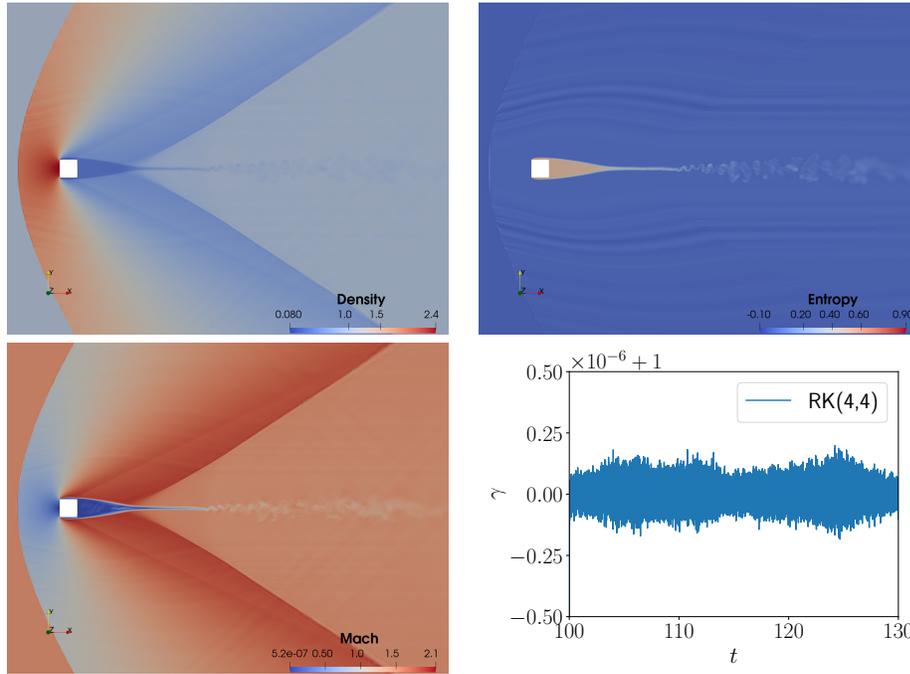


FIG. 13. Density, thermodynamic entropy, local Mach number contours and snapshot of the time evolution of the relaxation parameter,  $\gamma$ , for the supersonic flow around a square cylinder with  $Re_\infty = 10^4$  and  $M_\infty = 1.5$  at  $t = 130$ .

- primary conservative,
- entropy-conservative/entropy-stable in the fully discrete sense with  $\Delta t = \mathcal{O}(\Delta x)$ ,
- explicit, except for the solution of a scalar algebraic equation at each time step,
- arbitrarily high order accurate in space and time.

Furthermore, the added computational cost of this modification is insignificant in the context of typical computational fluid dynamics calculations. It is anticipated that this type of entropy stable formulation will begin to bear fruit for industrial simulations in the near future [44]. Finally, relaxation schemes provide an entropy guarantee without degrading solution accuracy or adding unnecessary dissipation.

Further desirable properties of fully discrete numerical methods for the compressible Euler and Navier–Stokes equations not studied in this article concern additional elements of robustness, e.g., preserving the positivity of two thermodynamic variables (e.g., density and pressure). To use the framework of [58], the interplay of limiters and relaxation schemes has to be studied.

Moreover, having a local entropy (in-)equality instead of the global one established in this article might be advantageous. However, this seems to be currently out of reach using the relaxation schemes proposed here. While fully discrete local entropy inequalities can be achieved by the addition of sufficient artificial viscosity, the advantage of relaxation schemes is that they do not impose excessive dissipation; if the baseline scheme is dissipative, they can even remove some of this dissipation.

**Acknowledgment.** We are thankful for the computing resources of the Supercomputing Laboratory and the Extreme Computing Research Center at King Abdulah University of Science and Technology.

## REFERENCES

- [1] S. ABHYANKAR, J. BROWN, E. M. CONSTANTINESCU, D. GHOSH, B. F. SMITH, AND H. ZHANG, *PETSc/TS: A Modern Scalable ODE/DAE Solver Library*, <https://arxiv.org/abs/1806.01437>, 2018.
- [2] S. BALAY, S. ABHYANKAR, M. F. ADAMS, J. BROWN, P. BRUNE, K. BUSCHELMAN, L. DALCIN, A. DENER, V. ELJKHOUT, W. D. GROPP, D. KAUSHIK, M. G. KNEPLEY, D. A. MAY, L. C. MCINNES, R. T. MILLS, T. MUNSON, K. RUPP, P. SANAN, B. F. SMITH, S. ZAMPINI, H. ZHANG, AND H. ZHANG, *PETSc Users Manual*, Technical report ANL-95/11 (revision 3.10), Argonne National Laboratory, 2018.
- [3] P. BOGACKI AND L. F. SHAMPINE, A 3 (2) *pair of Runge–Kutta formulas*, Appl. Math. Lett., 2 (1989), pp. 321–325, [https://doi.org/10.1016/0893-9659\(89\)90079-7](https://doi.org/10.1016/0893-9659(89)90079-7).
- [4] P. BOGACKI AND L. F. SHAMPINE, An efficient Runge–Kutta (4, 5) pair, Comput. Math. Appl., 32 (1996), pp. 15–28, [https://doi.org/10.1016/0898-1221\(96\)00141-1](https://doi.org/10.1016/0898-1221(96)00141-1).
- [5] R. P. BRENT, *Algorithms for Minimization Without Derivatives*, Ser. Automat. Comput., Prentice-Hall, Englewood Cliffs, NJ, 1973.
- [6] J. C. BUTCHER, *Numerical Methods for Ordinary Differential Equations*, John Wiley & Sons, Chichester, 2008.
- [7] M. CALVO, D. HERNÁNDEZ-ABREU, J. I. MONTIJANO, AND L. RÁNDEZ, On the preservation of invariants by explicit Runge–Kutta methods, SIAM J. Sci. Comput., 28 (2006), pp. 868–885, <https://doi.org/10.1137/04061979X>.
- [8] M. CALVO, M. LABURTA, J. MONTIJANO, AND L. RÁNDEZ, Projection methods preserving Lyapunov functions, BIT, 50 (2010), pp. 223–241, <https://doi.org/10.1007/s10543-010-0259-3>.
- [9] M. CALVO, M. LABURTA, J. I. MONTIJANO, AND L. RÁNDEZ, Runge–Kutta projection methods with low dispersion and dissipation errors, Adv. Comput. Math., 41 (2015), pp. 231–251, <https://doi.org/10.1007/s10444-014-9355-2>.
- [10] M. H. CARPENTER, T. C. FISHER, E. J. NIELSEN, AND S. H. FRANKEL, Entropy stable spectral collocation schemes for the Navier–Stokes equations: Discontinuous interfaces, SIAM J. Sci. Comput., 36 (2014), pp. B835–B867, <https://doi.org/10.1137/130932193>.
- [11] M. H. CARPENTER AND C. A. KENNEDY, Fourth-Order 2N Runge–Kutta Schemes, Technical report NASA-TM-109112, NASA, 1994, <https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/19940028444.pdf>.
- [12] M. H. CARPENTER, M. PARSANI, E. J. NIELSEN, AND T. C. FISHER, Towards an entropy stable spectral element framework for computational fluid dynamics, in Proceedings of the 54th AIAA Aerospace Sciences Meeting, AIAA 2016-1058, American Institute of Aeronautics and Astronautics, 2016.
- [13] C. M. DAFERMOS, *Hyperbolic Conservation Laws in Continuum Physics*, Springer-Verlag, Berlin, 2010.
- [14] L. DALCIN, D. B. ROJAS, S. ZAMPINI, D. C. DEL REY FERNÁNDEZ, M. H. CARPENTER, AND M. PARSANI, Conservative and entropy stable solid wall boundary conditions for the compressible Navier–Stokes equations: Adiabatic wall and heat entropy transfer, J. Comput. Phys., 397 (2019).
- [15] K. DEKKER AND J. G. VERWER, *Stability of Runge–Kutta Methods for Stiff Nonlinear Differential Equations*, CWI Monogr. 2, North-Holland, Amsterdam, 1984.
- [16] N. DEL BUONO AND C. MASTROSERIO, Explicit methods based on a class of four stage fourth order Runge–Kutta methods for preserving quadratic laws, J. Comput. Appl. Math., 140 (2002), pp. 231–243, [https://doi.org/10.1016/S0377-0427\(01\)00398-3](https://doi.org/10.1016/S0377-0427(01)00398-3).
- [17] D. C. D. R. FERNÁNDEZ, M. H. CARPENTER, L. DALCIN, L. FREDRICH, D. ROJAS, A. R. WINTERS, G. J. GASSNER, S. ZAMPINI, AND M. PARSANI, Entropy stable  $p$ -nonconforming discretizations with the summation-by-parts property for the compressible Euler equations, SIAM J. Sci. Comput., 2019, submitted.
- [18] D. C. D. R. FERNÁNDEZ, M. H. CARPENTER, L. DALCIN, L. FREDRICH, A. R. WINTERS, G. J. GASSNER, AND M. PARSANI, Entropy stable  $p$ -nonconforming discretizations with the summation-by-parts property for the compressible Navier–Stokes equations, Comput. & Fluids, 2019, submitted.
- [19] L. FRIEDRICH, G. SCHNÜCKE, A. R. WINTERS, D. C. D. R. FERNÁNDEZ, G. J. GASSNER, AND M. H. CARPENTER, Entropy stable space-time discontinuous Galerkin schemes with

- summation-by-parts property for hyperbolic conservation laws*, J. Sci. Comput., 80 (2019), pp. 175–222, <https://doi.org/10.1007/s10915-019-00933-2>.
- [20] S. GOTTLIEB, D. I. KETCHESON, AND C.-W. SHU, *Strong Stability Preserving Runge–Kutta and Multistep Time Discretizations*, World Scientific, Singapore, 2011.
- [21] V. GRIMM AND G. QUISPEL, *Geometric integration methods that preserve Lyapunov functions*, BIT, 45 (2005), pp. 709–723, <https://doi.org/10.1007/s10543-005-0034-z>.
- [22] E. HAIRER, C. LUBICH, AND G. WANNER, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer Ser. Comput. Math. 31, Springer-Verlag, Berlin, 2006, <https://doi.org/10.1007/3-540-30666-8>.
- [23] E. HAIRER, S. P. NØRSETT, AND G. WANNER, *Solving Ordinary Differential Equations I: Nonstiff Problems*, Springer Ser. Comput. Math. 8, Springer-Verlag, Berlin, 2008, <https://doi.org/10.1007/978-3-540-78862-1>.
- [24] I. HIGUERAS, *Monotonicity for Runge–Kutta methods: Inner product norms*, J. Sci. Comput., 24 (2005), pp. 97–117, <https://doi.org/10.1007/s10915-004-4789-1>.
- [25] E. JONES, T. OLIPHANT, P. PETERSON, ET AL., *SciPy: Open Source Scientific Tools for Python*, 2001, <http://www.scipy.org>.
- [26] D. I. KETCHESON, *Highly efficient strong stability-preserving Runge–Kutta methods with low-storage implementations*, SIAM J. Sci. Comput., 30 (2008), pp. 2113–2136, <https://doi.org/10.1137/07070485X>.
- [27] D. I. KETCHESON, *Relaxation Runge–Kutta methods: Conservation and stability for inner-product norms*, SIAM J. Numer. Anal., 57 (2019), pp. 2850–2870.
- [28] M. G. KNEPLEY AND D. A. KARPEEV, *Mesh algorithms for PDE with Sieve I: Mesh distribution*, Sci. Program., 17 (2009), pp. 215–230, <https://doi.org/10.3233/SPR-2009-0249>.
- [29] H. KOJIMA, *Invariants preserving schemes based on explicit Runge–Kutta methods*, BIT, 56 (2016), pp. 1317–1337, <https://doi.org/10.1007/s10543-016-0608-y>.
- [30] M. LABURTA, J. I. MONTIJANO, L. RÁNDEZ, AND M. CALVO, *Numerical methods for non conservative perturbations of conservative problems*, Comput. Phys. Commun., 187 (2015), pp. 72–82, <https://doi.org/10.1016/j.cpc.2014.10.012>.
- [31] P. G. LEFLOCH, J.-M. MERCIER, AND C. ROHDE, *Fully discrete, entropy conservative schemes of arbitrary order*, SIAM J. Numer. Anal., 40 (2002), pp. 1968–1992, <https://doi.org/10.1137/S003614290240069X>.
- [32] C. LOZANO, *Entropy production by explicit Runge–Kutta schemes*, J. Sci. Comput., 76 (2018), pp. 521–565, <https://doi.org/10.1007/s10915-017-0627-0>.
- [33] J. J. MORÉ, B. S. GARBOW, AND K. E. HILLSTROM, *User Guide for MINPACK-1*, Technical report ANL-80-74, Argonne National Laboratory, Argonne, Illinois, 1980.
- [34] P. ÖFFNER, J. GLAUBITZ, AND H. RANOCHA, *Analysis of artificial dissipation of explicit and implicit time-integration methods*, Int. J. Numer. Anal. Model., to appear.
- [35] M. PARSANI, M. H. CARPENTER, T. C. FISHER, AND E. J. NIELSEN, *Entropy stable staggered grid discontinuous spectral collocation methods of any order for the compressible Navier–Stokes equations*, SIAM J. Sci. Comput., 38 (2016), pp. A3129–A3162.
- [36] M. PARSANI, M. H. CARPENTER, AND E. J. NIELSEN, *Entropy stable discontinuous interfaces coupling for the three-dimensional compressible Navier–Stokes equations*, J. Comput. Phys., 290 (2015), pp. 132–138.
- [37] M. PARSANI, M. H. CARPENTER, AND E. J. NIELSEN, *Entropy stable wall boundary conditions for the three-dimensional compressible Navier–Stokes equations*, J. Comput. Phys., 292 (2015), pp. 88–113.
- [38] H. RANOCHA, *Shallow water equations: Split-form, entropy stable, well-balanced, and positivity preserving numerical methods*, GEM Int. J. Geomath., 8 (2017), pp. 85–133, <https://doi.org/10.1007/s13137-016-0089-9>.
- [39] H. RANOCHA, *On Strong Stability of Explicit Runge–Kutta Methods for Nonlinear Semibounded Operators*, 2018, <https://arxiv.org/abs/1811.11601>.
- [40] H. RANOCHA, J. GLAUBITZ, P. ÖFFNER, AND T. SONAR, *Stability of artificial dissipation and modal filtering for flux reconstruction schemes using summation-by-parts operators*, Appl. Numer. Math., 128 (2018), pp. 1–23, <https://doi.org/10.1016/j.apnum.2018.01.019>.
- [41] H. RANOCHA AND D. I. KETCHESON, *ConvexRelaxationRungeKutta. Relaxation Runge–Kutta Methods for Convex Functionals*, 2019 <https://github.com/ranocha/ConvexRelaxationRungeKutta>.
- [42] H. RANOCHA AND P. ÖFFNER, *L<sub>2</sub> stability of explicit Runge–Kutta schemes*, J. Sci. Comput., 75 (2018), pp. 1040–1056, <https://doi.org/10.1007/s10915-017-0595-4>.
- [43] C.-W. SHU AND S. OSHER, *Efficient implementation of essentially non-oscillatory shock-capturing schemes*, J. Comput. Phys., 77 (1988), pp. 439–471, [https://doi.org/10.1016/0021-9991\(88\)90177-5](https://doi.org/10.1016/0021-9991(88)90177-5).

- [44] J. SLOTNICK, A. KHODADOUST, J. ALONSO, D. DARMOFAL, W. GROPP, E. LURIE, AND D. MAVRIPLIS, *CFD Vision 2030 Study: A Path to Revolutionary Computational Aero-science*, NASA CR-2014-218178 (2014).
- [45] E. SÜLI AND D. F. MAYERS, *An Introduction to Numerical Analysis*, Cambridge University Press, Cambridge, 2003, <https://doi.org/10.1017/CBO9780511801181>.
- [46] Z. SUN AND C.-W. SHU, *Stability of the fourth order Runge–Kutta method for time-dependent partial differential equations*, *Ann. Math. Sci. Appl.*, 2 (2017), pp. 255–284, <https://doi.org/10.4310/AMSA.2017.v2.n2.a3>.
- [47] Z. SUN AND C.-W. SHU, *Strong stability of explicit Runge–Kutta time discretizations*, *SIAM J. Numer. Anal.*, 57 (2019), pp. 1158–1182.
- [48] M. SVÄRD AND H. ÖZCAN, *Entropy-stable schemes for the Euler equations with far-field and wall boundary conditions*, *J. Sci. Comput.*, 58 (2014), pp. 61–89.
- [49] E. TADMOR, *The numerical viscosity of entropy stable schemes for systems of conservation laws. I*, *Math. Comp.*, 49 (1987), pp. 91–103, <https://doi.org/10.1090/S0025-5718-1987-0890255-3>.
- [50] E. TADMOR, *From semidiscrete to fully discrete: Stability of Runge–Kutta schemes by the energy method II*, in *Collected Lectures on the Preservation of Stability under Discretization*, D. J. Estep and S. Tavener, eds., *Proc. Appl. Math.* 109, SIAM, Philadelphia, 2002, pp. 25–49.
- [51] E. TADMOR, *Entropy stability theory for difference approximations of nonlinear conservation laws and related time-dependent problems*, *Acta Numer.*, 12 (2003), pp. 451–512, <https://doi.org/10.1017/S0962492902000156>.
- [52] E. TADMOR AND W. ZHONG, *Entropy stable approximations of Navier–Stokes equations with no artificial numerical viscosity*, *J. Hyperbolic Differ. Equ.*, 3 (2006), pp. 529–559, <https://doi.org/10.1142/S0219891606000896>.
- [53] V. A. TITAREV AND E. F. TORO, *Finite volume WENO schemes for three-dimensional conservation laws*, *J. Comput. Phys.*, 201 (2014), pp. 238–260.
- [54] J. H. VERNER, *Explicit Runge–Kutta methods with estimates of the local truncation error*, *SIAM J. Numer. Anal.*, 15 (1978), pp. 772–790, <https://doi.org/10.1137/0715051>.
- [55] N. WINTERMEYER, A. R. WINTERS, G. J. GASSNER, AND D. A. KOPRIVA, *An entropy stable nodal discontinuous Galerkin method for the two dimensional shallow water equations on unstructured curvilinear meshes with discontinuous bathymetry*, *J. Comput. Phys.*, 340 (2017), pp. 200–242.
- [56] A. R. WINTERS AND G. J. GASSNER, *Affordable, entropy conserving and entropy stable flux functions for the ideal MHD equations*, *J. Comput. Phys.*, 304 (2016), pp. 72–108.
- [57] H. ZAKERZADEH AND U. S. FJORDHOLM, *High-order accurate, fully discrete entropy stable schemes for scalar conservation laws*, *IMA J. Numer. Anal.*, 36 (2016), pp. 633–654, <https://doi.org/10.1093/imanum/drv020>.
- [58] X. ZHANG AND C.-W. SHU, *Maximum-principle-satisfying and positivity-preserving high-order schemes for conservation laws: survey and new developments*, *Proc. Roy. A*, 467 (2011), pp. 2752–2776, <https://doi.org/10.1098/rspa.2011.0153>.