

Relaxation Runge–Kutta Methods: Fully-Discrete Explicit Entropy-Stable Schemes for the Euler and Navier–Stokes Equations

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The framework of inner product norm preserving relaxation Runge–Kutta methods (David I. Ketcheson, *Relaxation Runge–Kutta Methods: Conservation and Stability for Inner-Product Norms*, 2019. arXiv: 1905.09847 [math.NA]) 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 semi-discretizations 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

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1 Introduction

Consider a time-dependent ordinary differential equation (ODE)

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

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 η might represent e.g. some form of energy or momentum; in the present work we refer to η as *entropy*, with a view to applications in hyperbolic and incompletely parabolic system of partial differential equations (PDEs) such as the compressible Euler and Navier–Stokes equations. The time evolution of η is given by $\frac{d}{dt}\eta(u(t)) = \langle \eta'(u(t)), f(t, u(t)) \rangle$. Thus entropy *dissipative* systems satisfy

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

while entropy *conservative* ones fulfill

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

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 Runge–Kutta method.

In this work we focus on applications to entropy conservative or entropy dissipative semi-discretizations of hyperbolic conservation laws [46, 48] and the Navier–Stokes equations (incompletely parabolic); 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 η' 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 towards complete nonlinear and entropy stability of numerical algorithms because most of the research has been focused on semi-discrete schemes (see, for instance, [10, 17, 34, 36, 45, 51, 52]). Stability/dissipation results for fully discrete schemes have mainly been limited to semi-discretizations including certain amounts of dissipation [23, 37, 46, 53], linear equations [40, 43, 44, 47], or fully implicit time integration schemes [18, 30, 46]. For explicit methods and general equations, there are negative experimental and theoretical results concerning entropy stability [31, 35].

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 ordinary differential equations, and to both explicit and implicit Runge–Kutta 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 [21] and references therein.

The basic idea behind the methods proposed here comes from Dekker & Verwer [15, pp. 265–266] and has been developed for inner-product norms in [26]. The idea (and notation) of Dekker & Verwer [15] was applied in [16] to a restricted class of fourth order methods. This was extended in [8] by giving a general proof that applying the technique to a Runge–Kutta 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 a Runge–Kutta projection method where the search direction is the same as the direction of the next time step update. Nevertheless, the main focus in [8] is on a different type of projection in which the search direction is chosen based on an embedded method. Grimm & Quispel [20] extended the standard orthogonal projection method [21, Section IV.4] to dissipative systems possessing a Lyapunov function and the same approach was used in [7, 29] with the choice of search directions advocated in [8].

Kojima [28] reviewed some related methods and proposed another kind of projection scheme for conservative systems.

Like standard Runge–Kutta methods, and in contrast to orthogonal projection methods, the schemes based on the approach of Dekker & Verwer [15] or Calvo et al. [8] 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 [21, Section IV.4] and the type of projection or search direction [7, 9, 28, 38].

The goal of this article is to extend the theory developed in [26] 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. 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) Runge–Kutta method with s stages can be represented by its Butcher tableau [6, 22]

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

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

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

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

Here, y_i are the stage values of the Runge–Kutta method. We will make use of the shorthand

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

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

A Runge–Kutta 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* [23, 35].

2 Relaxation Runge–Kutta Methods

Following [15, pp. 265–266] and [26], the basic idea to make a given Runge–Kutta method entropy stable is to scale the weights b_i by a parameter $\gamma_n \in \mathbb{R}$, i.e. to use

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

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 γ_n proposed in [26] is such that

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

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

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

by finding a root γ_n of

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

Note that the direction

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

and the estimate of the entropy change

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

can be computed on the fly during the computation of the Runge–Kutta method and are not influenced by γ_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 semi-discretization of a (hyperbolic) PDE with entropy S and entropy variables $w(u) = S'(u)$ in the domain Ω , (2.4) corresponds to a discrete version of

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

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

If f is a semi-discretization of a PDE and η the global entropy, $r(\gamma = 1)$ can be interpreted as global entropy production of the unmodified Runge–Kutta 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 [26, Theorem 2.1], which dealt only with inner-product norms.

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

The new numerical solution u_γ^{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 [26], the given Runge–Kutta method determines the direction d and γ_n can be interpreted as a relaxation parameter determined by the requirement of preserving the evolution of η . Hence, the method defined by (1.5a) & (2.1) with the interpretation $u_\gamma^{n+1} \approx u(t_n + \gamma_n \Delta t)$ is called a *relaxation Runge–Kutta* (RRK) method. The scheme using $u_\gamma^{n+1} \approx u(t_n + \Delta t)$ will be referred to as an IDT method [8].

2.1 Existence of a Solution

Obviously, $r(0) = 0$ and r is convex since the entropy η 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 2.3. *Let a Runge–Kutta 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 definition of r (2.4),

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

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

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

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

Remark 2.4. The assumption $\sum_{i=1}^s b_i a_{ij} > 0$ is satisfied for all (at least) second order accurate Runge–Kutta methods since $\sum_{i=1}^s b_i a_{ij} = 1/2$ is a condition for second-order accuracy.

Lemma 2.5. *Let a Runge–Kutta 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),

$$\begin{aligned} r'(1) &= \Delta t \sum_{i=1}^s b_i \langle \eta'(u^{n+1}), f_i \rangle - \Delta t \sum_{i=1}^s b_i \langle \eta'(y_i), f_i \rangle \\ &= -\Delta t \sum_{i=1}^s b_i \int_0^1 \eta''\left(u^{n+1} + v \Delta t \sum_{k=1}^s (a_{ik} - b_k) f_k\right) \left(f_i, \Delta t \sum_{j=1}^s (a_{ij} - b_j) f_j\right) dv. \end{aligned} \quad (2.10)$$

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

$$r'(1) = -\Delta t^2 \sum_{i,j=1}^s b_i (a_{ij} - b_j) \int_0^1 \eta''\left(u^{n+1} + v \Delta t \sum_{k=1}^s (a_{ik} - b_k) f_k\right) (f_0, f_0) dv + \mathcal{O}(\Delta t)^3. \quad (2.11)$$

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

Remark 2.6. The assumption $\sum_{i,j=1}^s b_i (a_{ij} - b_j) < 0$ is satisfied for all (at least) second order accurate Runge–Kutta methods since $\sum_{i,j=1}^s b_i (a_{ij} - b_j) = 1/2 - 1 = -1/2$ in that case.

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

Theorem 2.7. *Assume that the Runge–Kutta 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 . \square

Remark 2.8. The value $\eta''(u^n)(f_0, f_0)$ of the quadratic form $\eta''(u^n)$ is positive for a strictly convex entropy η if $f_0 \neq 0$. If $f_0 = 0$ and the system is autonomous, every explicit Runge–Kutta method will yield a stationary solution. The results of Lemmas 2.3 & 2.5 and hence of Theorem 2.7 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 2.9. The proof of Theorem 2.7 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 γ_n (if the assumptions of Theorem 2.7 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. However, the following result has been obtained in [26, Theorem 2.4].

Theorem 2.10. *Let the given Runge–Kutta method be of order p . Consider the IDT/RRK method defined by (1.5a) & (2.1) and suppose that $\gamma_n = 1 + O(\Delta t^{p-1})$.*

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 initial value for u at t_n , a Runge–Kutta method with order of accuracy p yields

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

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 Runge–Kutta order conditions guarantee

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

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

Theorem 2.11. *Let W be a Banach space, $\psi: [0, T] \times \mathcal{H} \rightarrow W$ a smooth function, and b_i, c_i coefficients of a Runge–Kutta method of order p . Then*

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

Corollary 2.12. *If η is smooth and the given Runge–Kutta method is p -th order accurate, $r(\gamma = 1) = O(\Delta t^{p+1})$.*

Proof of Corollary 2.12. Apply Theorem 2.11 to $\psi(t, u) = \langle \eta'(u), f(t, u) \rangle$ and use (2.12), resulting in

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

□

Proof of Theorem 2.11. Consider $\phi(t) = \int_{t_n}^t \psi(\tau, u(\tau)) d\tau$. Applying the Runge–Kutta method to the extended ODE (with a slight abuse of notation)

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

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

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

Additionally,

$$\phi(t_n + \Delta t) = \int_{t_n}^{t_n + \Delta t} \psi(t, u(t)) dt = \Delta t \sum_{i=1}^s b_i \psi(t_n + c_i \Delta t, u(t_n + c_i \Delta t)) + \mathcal{O}(\Delta t^{p+1}). \quad (2.18)$$

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

Remark 2.13. Theorem 2.11 can be seen as a superconvergence result for integrals evaluated using the quadrature rule associated with a Runge–Kutta method.

Theorem 2.14. Assume that the conditions of Theorem 2.7 are satisfied. Hence, there exists a unique positive root γ_n of r (2.4). Consider the IDT/RRK method defined by (1.5a) & (2.1) and suppose that the given Runge–Kutta method is p -th order accurate.

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

Proof. Because of Corollary 2.12, $r(1) = \mathcal{O}(\Delta t^{p+1})$. As can be seen in the proof of Lemma 2.5, $r'(1) = c\Delta t^2 + \mathcal{O}(\Delta t^3)$, where $c > 0$. Hence, there is a root $\gamma_n = 1 + \mathcal{O}(\Delta t^{p-1})$ of r (2.4). Applying Theorem 2.10 yields the desired accuracy result. \square

Remark 2.15. As an extension of Remark 2.9, the behavior of the temporal entropy dissipation r (2.4) can be described as follows for sufficiently small Δt if the assumptions of Theorem 2.7 are satisfied: Firstly, $r(0) = 0$, $r(1) = \mathcal{O}(\Delta t^{p+1}) \approx 0$, 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 γ_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 1a for a typical plot of $r(\gamma)$.

2.3 Additional Properties and Generalizations

As described in [26], relaxation RK methods still conserve linear invariants, although γ_n is determined in a nonlinear way. Such linear invariants are e.g. the total mass for a semi-discretization 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 [19] and references cited therein. It has been shown in [26, Section 3] that the relaxation modification of many SSP methods retains the same SSP property of the original method as long as γ_n deviates not too much from unity.

If there are several convex quantities η_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 η_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 2.15.

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

Proposition 2.16. *Suppose that the given Runge–Kutta method is p -th order accurate with $p \geq 2$. If $\langle \eta'(u^{n+1}), \sum_{i=1}^s b_i f_i \rangle / \|\sum_{i=1}^s b_i f_i\| = B(u^n)\Delta t + O(\Delta t^2)$ with $B(u^n) \neq 0$, then r (2.4) has a positive root $\gamma_n = 1 + O(\Delta t^{p-1})$. If this root is used to define IDT/RRK methods by (1.5a) & (2.1), then:*

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 [7, Theorem 2] using the implicit function theorem can be adapted to this setting; the normalized search direction considered there is $w = d/\|d\|$ and the projected value is $u_\gamma^{n+1} = u^{n+1} + (1 - \gamma_n)d = u^{n+1} + \lambda_n w$, i.e. the step parameters are related via $\gamma_n = 1 + \lambda_n/\|d\|$. Since there is a solution $\lambda_n = O(\Delta t^p)$ and $d = \Delta t \sum_{i=1}^s b_i f_i$ scales as Δt , there is a solution $\gamma_n = 1 + O(\Delta t^{p-1})$. Applying Theorem 2.10 yields the desired results. \square

Remark 2.17. While Proposition 2.16 can be applied to general functions η , 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 γ_n) are useful for applications and root finding procedures.

2.4 Implementation

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

$$r'(\gamma) = \langle \eta'(u^n + \gamma d), d \rangle - e, \quad (2.19)$$

where the direction d 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 [32]) from SciPy [24] 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 γ is chosen as initial guess, since γ changes only slightly from step to step. Implementations used for the numerical examples up to section 3.4 are provided in [39].

3 Numerical Examples

The following Runge–Kutta methods with weights $b_i \geq 0$ will be used in the numerical experiments. The value of Δt is fixed in each test and embedded error estimators are not used.

- SSPRK(2,2): Two stage, second order SSP method of [41].
- SSPRK(3,3): Three stage, third order SSP method of [41].
- SSPRK(10,4): Ten stage, fourth order SSP method of [25].

- RK(4,4): Classical four stage, fourth order method.
- BSRK(8,5): Eight stage, fifth order method of [3].
- VRK(9,6): Nine stage, sixth order method of the family developed in [50]¹.
- VRK(13,8): Thirteen stage, eighth order method of the family developed in [50]².

3.1 Conserved Exponential Entropy

Consider the system

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

with exponential entropy

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

which is conserved for the analytical solution

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

The shape of $r(\gamma)$ for the first time step using SSPRK(3,3) is shown in Figure 1a. In accordance with the description given in Remark 2.15, $r(0) = 0$, $r(1) \approx 0$, r is negative between its roots and positive outside of this interval. The order of accuracy $r(1) = O(\Delta t^{p+1})$ guaranteed by Corollary 2.12 is obtained for the methods shown in Figure 1b.

Results of a convergence study in this setup are shown in Figure 2. 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 2.14. The IDT methods ($u_\gamma^{n+1} \approx u(t^n + \Delta t)$) yield a reduced order of convergence according to Theorem 2.14. 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 2c. Hence, the relaxation schemes are far superior in this case.

3.2 Dissipated Exponential Entropy

Consider the system

$$\frac{d}{dt} \begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} = \begin{pmatrix} -\exp(u_1(t)) \\ -\exp(u_2(t)) \end{pmatrix}, \quad u^0 = \begin{pmatrix} 1 \\ 0.5 \end{pmatrix}, \quad (3.4)$$

with exponential entropy (3.2), which is dissipated for the analytical solution

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

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 less problems for small Δt . Nevertheless, the order of convergence using the RRK schemes is still better than for the IDT methods, as explained by Theorem 2.14.

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

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

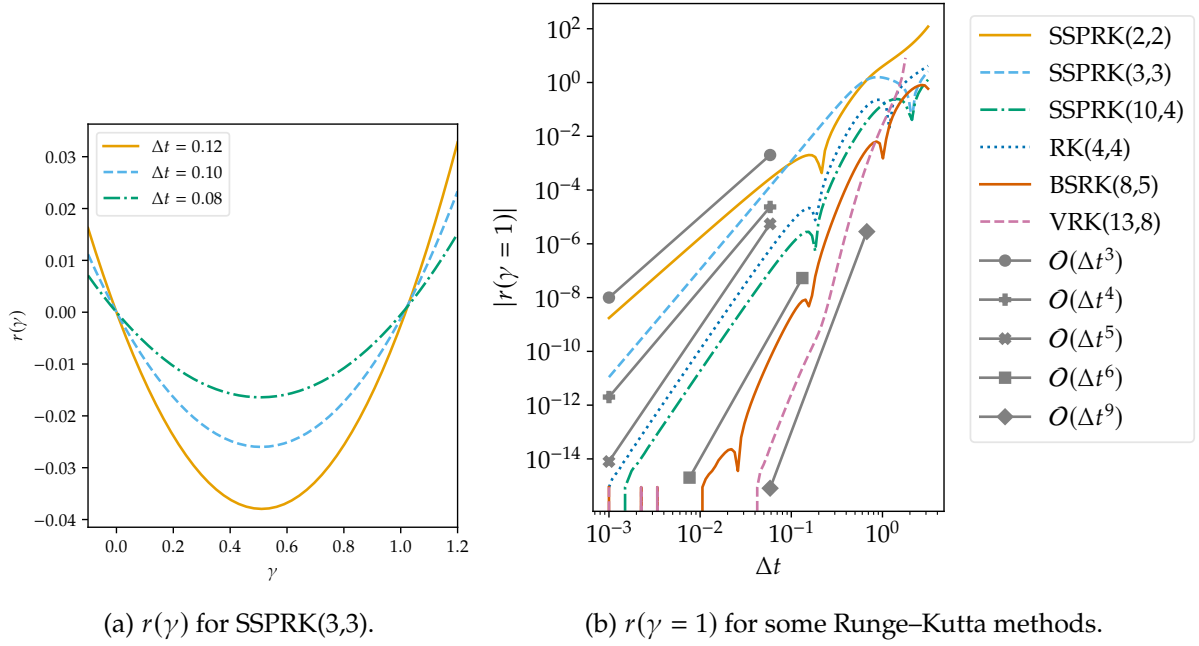


Figure 1: Numerical results for the temporal entropy production r (2.4) at the first time step for the entropy conservative ODE (3.1).

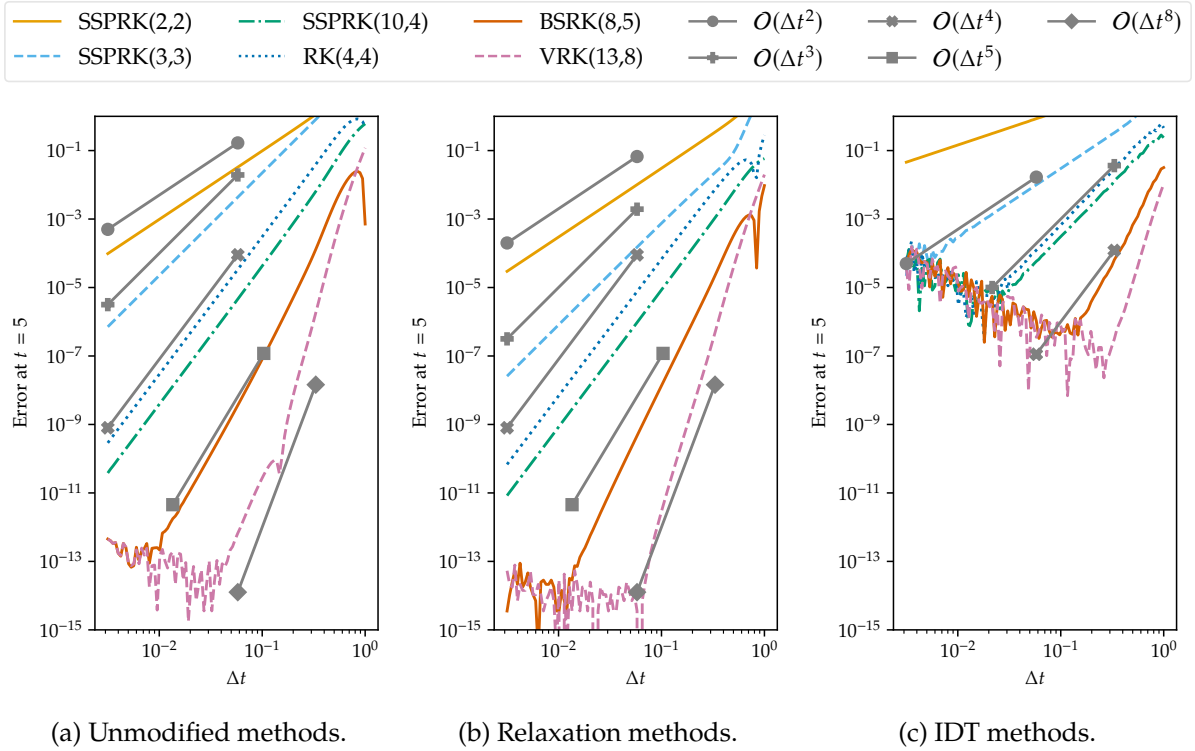


Figure 2: Convergence study for the entropy conservative ODE (3.1) with unmodified methods, RRK schemes ($u_\gamma^{n+1} \approx u(t^n + \gamma_n \Delta t)$), and IDT methods ($u_\gamma^{n+1} \approx u(t^n + \Delta t)$).

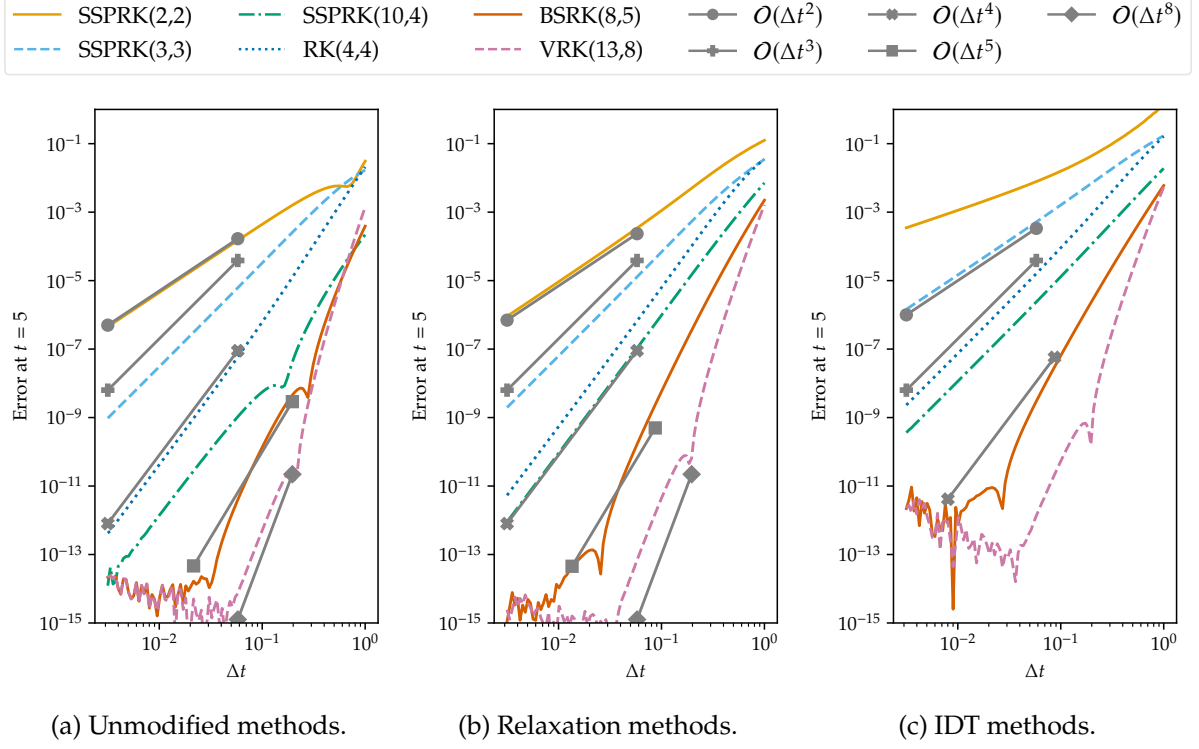


Figure 3: Convergence study for the entropy dissipative ODE (3.4) with unmodified methods, RRK schemes ($u_\gamma^{n+1} \approx u(t^n + \gamma_n \Delta t)$), and IDT methods ($u_\gamma^{n+1} \approx u(t^n + \Delta t)$).

3.3 Nonlinear Pendulum

Consider the system

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

with non-quadratic energy

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

which is conserved and convex as long as $|u_1| < \pi/2$.

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.

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 towards 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 [39].

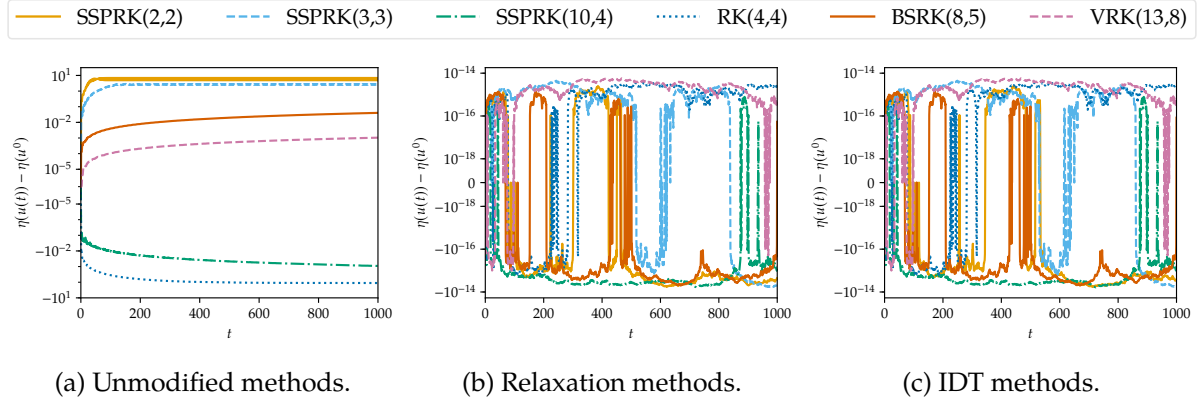


Figure 4: Evolution of the non-quadratic energy (3.7) of numerical solutions for the nonlinear pendulum (3.6).

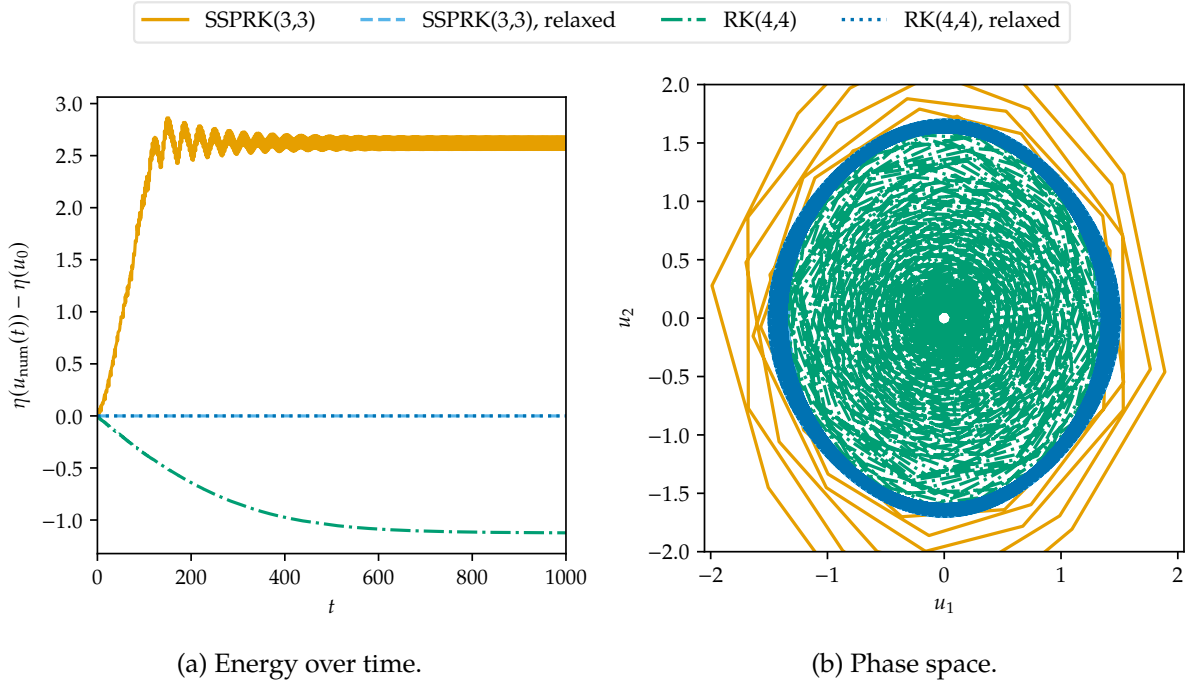


Figure 5: Numerical solutions for the nonlinear pendulum (3.6) using the unmodified and relaxation versions of SSPRK(3,3) and RK(4,4) with $\Delta t = 0.9$.

3.5 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

$$\begin{aligned} \frac{\partial \mathbf{Q}}{\partial t} + \sum_{m=1}^3 \frac{\partial \mathcal{F}_{x_m}^{(I)}}{\partial x_m} &= \sum_{m=1}^3 \frac{\partial \mathcal{F}_{x_m}^{(V)}}{\partial x_m}, \quad \forall (x_1, x_2, x_3) \in \Omega, \quad t \geq 0, \\ \mathbf{Q}(x_1, x_2, x_3, t) &= \mathcal{G}^{(B)}(x_1, x_2, x_3, t), \quad \forall (x_1, x_2, x_3) \in \Gamma, \quad t \geq 0, \\ \mathbf{Q}(x_1, x_2, x_3, 0) &= \mathcal{G}^{(0)}(x_1, x_2, x_3, 0), \quad \forall (x_1, x_2, x_3) \in \Omega. \end{aligned} \quad (3.8)$$

The vectors \mathbf{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 (3.8) by setting $\mathcal{F}_{x_m}^{(V)} = 0$.

It is well known that the compressible Navier–Stokes equations (3.8) possess a convex extension that, when integrated over the physical domain Ω , only depends on the boundary data on Γ . Such an extension yields the entropy function

$$S = -\rho s, \quad (3.9)$$

where ρ 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, 49].

Following the analysis described in [10, 11, 17, 34], we multiply multiply the PDE (3.8) by the (local) entropy variables $\mathbf{W} = \partial S / \partial \mathbf{Q}$ and arrive at the the integral form of the (scalar) entropy equation

$$\frac{d}{dt} \int_{\Omega} S d\Omega = \frac{d}{dt} \eta \leq \sum_{m=1}^3 \int_{\Gamma} \left(\mathbf{W}^T \mathcal{F}_{x_m}^{(V)} - \mathcal{F}_{x_m} \right) n_{x_m} d\Gamma - DT, \quad (3.10)$$

where n_{x_m} is the m -th component of the outward facing unit normal to Γ and

$$DT = \sum_{m,j=1}^3 \int_{\Omega} \left(\frac{\partial \mathbf{W}}{\partial x_m} \right)^T \mathbf{C}_{m,j} \frac{\partial \mathbf{W}}{\partial x_j} d\Omega. \quad (3.11)$$

We remark that viscous dissipation always introduces a negative rate of change in entropy, since the $-DT$ term in (3.10) is negative semi-definite. An increase in entropy within the domain can only result from data that convects or diffuses through the boundary Γ . For smooth flows, we note that the inequality sign in (3.10) becomes an equality. Finally, we highlight that the integral form of the entropy equation for the compressible Euler equations can be obtained from (3.10) 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 Ω with boundary Γ into non-overlapping hexahedral elements and we discretize the spatial terms using a multi-dimensional summation-by-parts simultaneous-approximation-terms (SBP-SAT) operator as described in [11, 17, 34], 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, 11, 34], the total entropy of the spatial discretization satisfies

$$\frac{d}{dt} \mathbf{1}^T \widehat{\mathbf{P}} \mathbf{S} = \frac{d}{dt} \eta = \mathbf{B}\mathbf{T} - \mathbf{D}\mathbf{T} + \Upsilon. \quad (3.12)$$

This equation mimics at the semi-discrete level each term in (3.10). Here \mathbf{BT} is the discrete boundary term (i.e., the discrete version of the first integral term on the right-hand side of (3.10)), \mathbf{DT} is the discrete dissipation term (i.e., the discrete version of the second term on the right-hand side of (3.10)) and \mathbf{Y} enforces interface coupling and boundary conditions [10, 11, 34]. 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, three 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 test case is the laminar flow in a lid-driven cavity where a non-zero 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, non-homogeneous boundary conditions are imposed.

The error is computed using the following norms:

$$\begin{aligned} \text{Discrete } L^1 : \quad \|q\|_{L^1} &= |\Omega|^{-1} \sum_{j=1}^{N_{el}} \mathbf{1}^\top \mathbf{P}_j \mathbf{J}_j \text{abs}(q_j), \\ \text{Discrete } L^2 : \quad \|q\|_{L^2}^2 &= |\Omega|^{-1} \sum_{j=1}^{N_{el}} q_j^\top \mathbf{P}_j \mathbf{J}_j q_j, \\ \text{Discrete } L^\infty : \quad \|q\|_{L^\infty} &= \max_{j=1 \dots N_{el}} \text{abs}(q_j). \end{aligned} \tag{3.13}$$

Here \mathbf{J}_j is the metric Jacobian of the curvilinear transformation from physical space to computational space of the j -th hexahedral element, N_{el} is the total number of hexahedral elements in the mesh and $|\Omega|$ is the volume of the domain.

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) [27] and scalable ordinary differential equation (ODE)/differential algebraic equations (DAE) solver library [1]. The parameter γ_n of the relaxation Runge–Kutta schemes is computed from Equation (2.4) to machine precision using the bisection method which, for efficiency, is implemented directly in the unstructured grid solver.

3.5.1 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

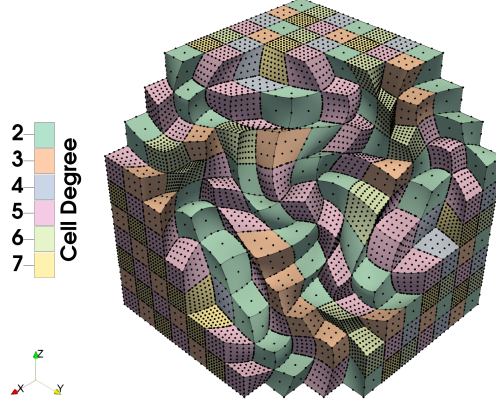


Figure 6: Isentropic vortex: mesh cut and polynomial degree distribution with non-conforming interfaces; $p = 2$ to $p = 7$.

problem is

$$\begin{aligned}
 \mathcal{G} &= 1 - \left\{ \left[(x_1 - x_{1,0}) - U_\infty \cos(\alpha) t \right]^2 + \left[(x_2 - x_{2,0}) - U_\infty \sin(\alpha) t \right]^2 \right\}, \\
 \rho &= T^{\frac{1}{\gamma-1}}, \quad T = \left[1 - \epsilon_v^2 M_\infty^2 \frac{\gamma-1}{8\pi^2} \exp(\mathcal{G}) \right], \\
 \mathcal{U}_1 &= U_\infty \cos(\alpha) - \epsilon_v \frac{(x_2 - x_{2,0}) - U_\infty \sin(\alpha) t}{2\pi} \exp\left(\frac{\mathcal{G}}{2}\right), \\
 \mathcal{U}_2 &= U_\infty \sin(\alpha) - \epsilon_v \frac{(x_1 - x_{1,0}) - U_\infty \cos(\alpha) t}{2\pi} \exp\left(\frac{\mathcal{G}}{2}\right), \quad \mathcal{U}_3 = 0,
 \end{aligned} \tag{3.14}$$

where U_∞ is the modulus of the free-stream velocity, M_∞ is the free-stream Mach number, c_∞ 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: $U_\infty = M_\infty c_\infty$, $\epsilon_v = 5$, $M_\infty = 0.5$, $\gamma = 1.4$, $\alpha = 45^\circ$, 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 (3.14) 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^∞ norms for fourth-, fifth-, 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 non-conforming 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].³ All the dissipation terms used for the interface coupling [17, 33] 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.

³This 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 relaxation Runge–Kutta 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^∞ Error	L^∞ 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

In addition to the Runge–Kutta methods mentioned at the beginning of Section 3, we use the following methods, that also have weights $b_i \geq 0$. Again, the value of Δt is fixed in each test, and embedded error estimators are not used.

- LCKRK(5,4): Five stage, fourth order method of [12].
- BSRK(3,3): Three stage, third order method of [4].
- BSRK(7,5): Seven stage, fifth order method of [3].
- VRK(10,7): Ten stage, seventh order method of the family developed in [50]⁴.

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.

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

$$\alpha \mathcal{V} \frac{\partial \mathcal{V}}{\partial x_1} - (\mathcal{V} - 1)(\mathcal{V} - \mathcal{V}_f) = 0; \quad -\infty \leq x_1 \leq +\infty, \quad t \geq 0, \quad (3.15)$$

whose solution can be written implicitly as

$$x_1 - \frac{1}{2} \alpha \left(\log |(\mathcal{V}(x_1) - 1)(\mathcal{V}(x_1) - \mathcal{V}_f)| + \frac{1 + \mathcal{V}_f}{1 - \mathcal{V}_f} \log \left| \frac{\mathcal{V}(x_1) - 1}{\mathcal{V}(x_1) - \mathcal{V}_f} \right| \right) = 0. \quad (3.16)$$

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

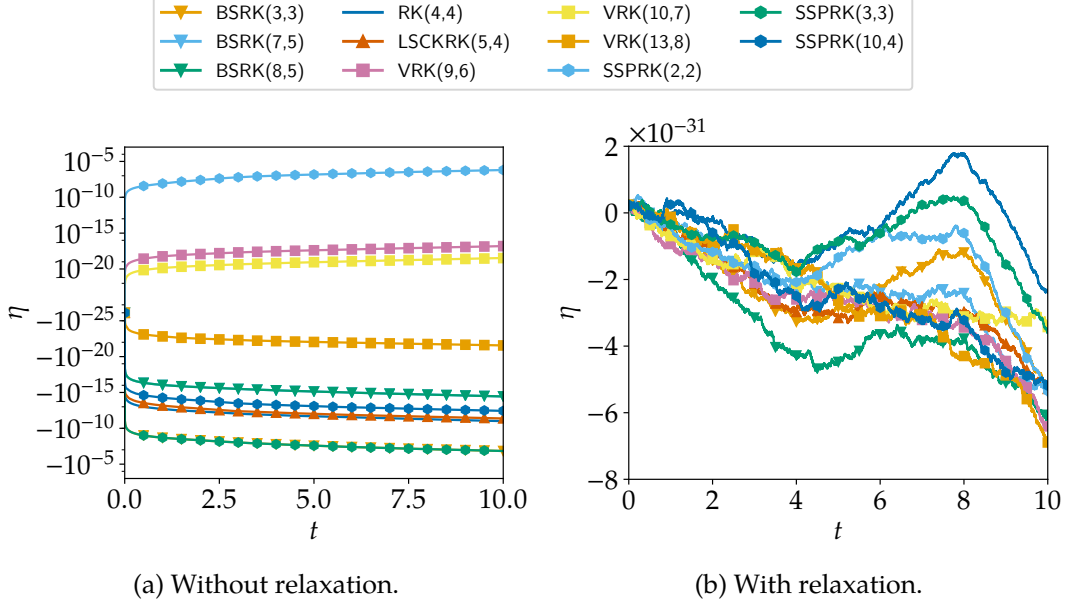


Figure 7: Isentropic vortex: time evolution of total entropy, using the spatial discretization shown in Figure 6.

where

$$\mathcal{V}_f \equiv \frac{\mathcal{U}_L}{\mathcal{U}_R}, \quad \alpha \equiv \frac{2\gamma}{\gamma+1} \frac{\mu}{Pr\dot{M}}. \quad (3.17)$$

Here $\mathcal{U}_{L/R}$ are known velocities to the left and right of the shock at $-\infty$ and $+\infty$, respectively, \dot{M} is the constant mass flow across the shock, Pr is the Prandtl number, and μ 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 Equation (3.16) 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.

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^∞ 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.

3.5.3 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 ω (see Figure 9b). 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

Table 2: Convergence study for the viscous shock using entropy stable SBP-SAT schemes with different solution polynomial degrees p and relaxation Runge–Kutta 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^∞ Error	L^∞ 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

terms used for the interface coupling [33] 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 relaxation Runge–Kutta schemes for the case where entropy conservative adiabatic wall boundary conditions [14] are used on all the six faces of the cavity (see Figure 8b). Figure 8a 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 a 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 8a. 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 relaxation Runge–Kutta schemes are shown. After a very short transient phase associated with the impulsive startup of the rotating plate, η decreases 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 Equation (3.12) which is non-zero is $-\mathbf{D}\mathbf{T}$. This contribution is strictly negative semi-definite and constant because the flow at this Reynolds number is laminar and steady and therefore, the gradient of the entropy variables in Equation (3.11) 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 8a. 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 stabilization 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 9a the results for the same set of relaxation Runge–Kutta schemes when a non-zero heat entropy flux, $g(t) = -10^{-4} \sin(4\pi t)$, is imposed on one of the faces adjacent to the rotating face (see Figure 9b). 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 a eighth-order accurate spatial scheme ($p = 7$) with the BSRK(8,5) and the VRK(9,6)

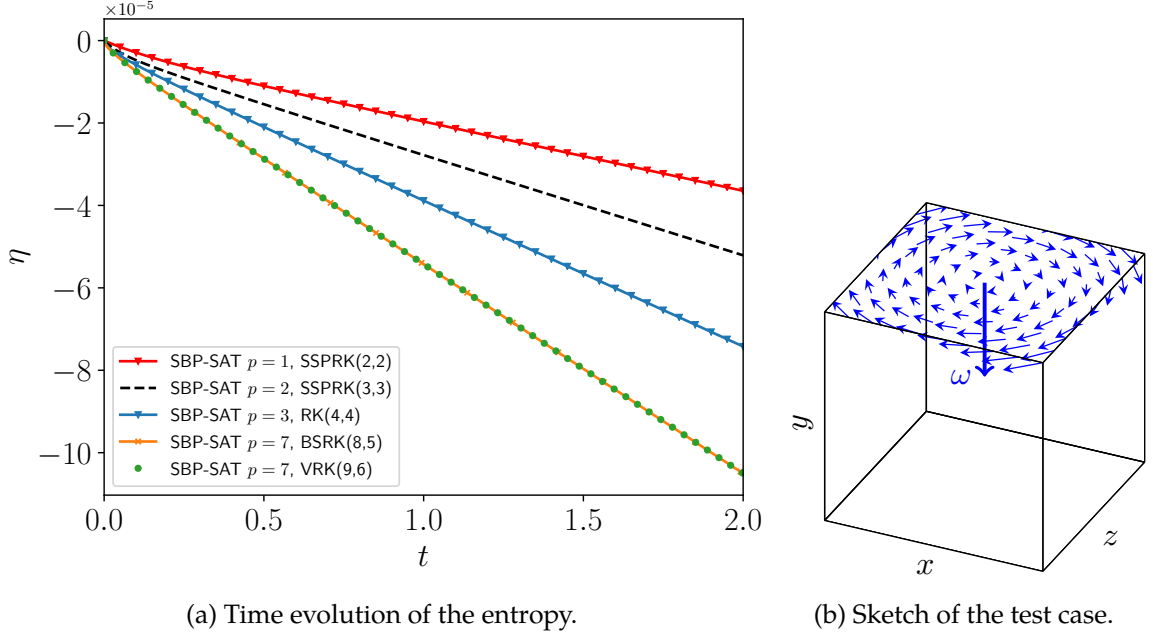


Figure 8: Driven cavity with rigid body rotation ω and zero heat entropy flux.

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 Conclusions

In this paper we have proposed, analyzed, and demonstrated a general approach which allows any Runge–Kutta 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 deeper 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 semi-discretization on unstructured grids, yields the *first discretization for computational fluid dynamics* that is:

- Primary conservative
- Entropy-conservative/entropy-stable in the fully-discrete sense with $\Delta t = O(\Delta x)$
- 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 novel entropy stable formulations will begin to bear fruit for industrial simulations in the near future [42].

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 robust-

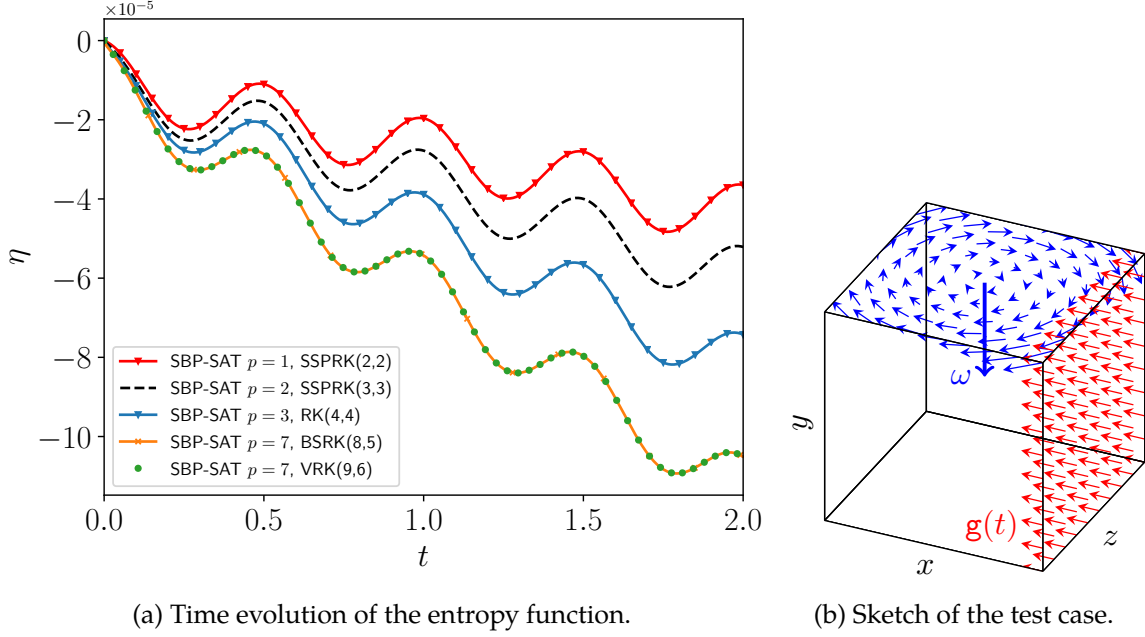


Figure 9: Driven cavity with rigid body rotation ω and non-zero heat entropy flux, $g(t)$.

ness, e.g. preserving the positivity of density and pressure. To use the framework of [54], 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.

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