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STRUCTURE-PRESERVING EXPONENTIAL RUNGE–KUTTA METHODS*

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Abstract. Exponential Runge–Kutta (ERK) and partitioned exponential Runge–Kutta (PERK) methods are developed for solving initial value problems with vector fields that can be split into conservative and linear nonconservative parts. The focus is on linearly damped ordinary differential equations that possess certain invariants when the damping coefficient is zero, but, in the presence of constant or time-dependent linear damping, the invariants satisfy linear differential equations. Similar to the way that Runge–Kutta and partitioned Runge–Kutta methods preserve quadratic invariants and symplecticity for Hamiltonian systems, ERK and PERK methods exactly preserve conformal symplecticity, as well as decay (or growth) rates in linear and quadratic invariants, under certain constraints on their coefficient functions. Numerical experiments illustrate the higher-order accuracy and structure-preserving properties of various ERK methods, demonstrating clear advantages over classical conservative Runge–Kutta methods, as well as usefulness for solving a wide range of differential equations.

Key words. structure-preserving algorithm, conformal symplectic, time-dependent damping, exponential integrators, integrating factor methods, exponential time differencing

AMS subject classifications. 65P10, 70F40, 37L50, 37M15

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1. Introduction.

Structure-preserving discretizations of a differential equation have solutions that satisfy certain properties that are also satisfied by exact solutions of the differential equation. It is well known that Runge–Kutta (RK) and partitioned Runge–Kutta (PRK) methods preserve quadratic invariants and symplecticity under certain conditions [10, 17, 28, 29, 31]. Thus, these methods are popular for solving conservative ODEs, because they approximate solutions with arbitrarily high orders of accuracy and, at the same time, produce qualitatively correct solution behavior. These methods and their structure-preserving properties have since been generalized or extended in various ways, including methods for solving oscillatory equations [4, 33], conservative PDEs [22, 27], Poisson systems [7], as well as energy-conserving schemes for Hamiltonian systems [6], just to name a few. Our focus is on developing structure-preserving RK-type methods for conservative ODEs that are perturbed by a linear, possibly time-dependent, damping term.

Previous work on this topic has developed several first- and second-order methods that preserve various properties of the governing equations. Sun and Shang [30] and Kong, Wu, and Mei [14] have proposed and analyzed methods, focusing on a first-order exponential implicit midpoint type method, that preserve a Birkhoffian symplectic structure. The work of Modin and Söderlind [24] and Bhatt, Floyd, and Moore [2] constructed and examined second-order exponential integrators (based on the implicit midpoint and Störmer–Verlet methods) for solving conformal Hamiltonian systems [19], which exactly preserve the contraction in the symplectic two-form, as well as several other dissipative properties. Similar work has proposed

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first-order exponential integrators, based on the symplectic Euler [25] and Preissmann [26] box schemes, which preserve the contraction of total symplecticity for dissipatively perturbed Hamiltonian PDEs. Many of these methods were constructed as splitting methods using the approach proposed by McLachlan and Quispel [20, 21]. Of course, higher-order methods can also be constructed using splitting techniques, but this approach can be tedious in practice, and obtaining proper order conditions is not always straightforward.

In this article, we present a simple approach to constructing higher-order integrators, known throughout the literature as exponential Runge–Kutta (ERK) and partitioned exponential Runge–Kutta (PERK) methods, which preserve various properties that are discussed in the aforementioned previous works. To be clear, our purpose is not to derive order conditions, but we rely on the fact that order conditions in many cases are known, based on derivation of the methods from standard RK methods using a Lawson transformation, or through analysis using B-series and bicolored rooted trees [1]. Our focus is, however, to find the restrictions on the coefficient functions of the methods that imply numerical structure preservation. Indeed, structure-preserving properties of some ERK and PERK methods have been considered in other previous works (see, for example, [5, 9]), and the structure-preserving properties of exponentially fitted RK methods presented in [4, 32] are analogous to some of the results of the present article. Yet, the results of those works are not applicable to the damped equations in which we are interested.

ERK methods have been developed for systems of equations with stiff linear terms [8, 15, 16], and they have demonstrated remarkable advantages for such problems. The exponential function in the methods provides the exact solution of the linear part, so the stiffness does not restrict the step size, and solutions to the nonlinear part may be approximated explicitly. As a result, ERK methods are often explicit, and there is usually no motivation for constructing or analyzing implicit ERK methods. Our focus, however, is different. We are concerned with equations that are damped (often weakly) by a linear part of the vector field but are otherwise conservative when that linear part is zero. Thus, there are certain advantages to solving the nonlinear part with a conservative method, so the ERK methods that we consider may or may not be implicit.

ERK methods have attracted a significant amount of attention in the past few decades. For a review of the research done on this method, see the unpublished manuscript [23] and references therein. Two types of ERK methods of particular interest are integrating factor (IFRK) methods and exponential time differencing (ETDRK) methods, but for the purpose of structure preservation we need not be restricted to either one of these classes, and we may even allow others. Linear stability analysis of ERK methods has also been investigated in some specific cases (see, for example, [9, 18]), but we find a stability result analogous to that of symplectic methods.

Altogether, our main contributions are as follows:

- We present a general formulation of ERK methods (section 2).
  - This formulation is applicable to equations with time-dependent linear coefficients.
  - This formulation provides new (previously unknown) structure-preserving algorithms.
- We prove structure preservation under certain restrictions on the coefficients of the methods.
  - The methods exactly preserve contractions in linear and quadratic quantities that are invariants in the absence of damping (section 3).

  - The methods exactly preserve conformal symplecticity, and the real part of the eigenvalues for linear equations (section 4).
- We provide numerical demonstrations of schemes in this class of ERK methods (section 5).
  - This initiation of exponential-time-differencing and higher-order conformal symplectic methods illustrates advantages over standard methods.
  - Application to a damped Poisson system provides a first look at numerical solution behavior for a system with conservative part that is not canonical Hamiltonian.

2. Exponential Runge–Kutta methods. Consider the following initial value problem:

$$\dot{z}(t) = N(z(t)) - \gamma(t)z(t), \quad z(0) = z_0, \tag{1}$$

where $z \in \mathbb{R}^d$ with $d \in \mathbb{N}$, $N : \mathbb{R}^d \to \mathbb{R}^d$ is a smooth nonlinear function of z, and $\dot{z}$ denotes the derivative of z with respect to t. ERK methods make use of a vector field that has been decomposed into linear and nonlinear parts, producing algorithms that have demonstrated many strengths for equations of the form (1). Typically, discussions on ERK methods take γ to be a constant matrix of compatible dimensions, but for our purposes we require that γ be scalar, and we allow it to depend on time, i.e., $\gamma(t) : \mathbb{R} \to \mathbb{R}$.

Following the approach designed by Lawson [16], define the change of variables (like a Lawson transformation)

$$y(t) = e^{x_0(t)}z(t) \qquad \text{with} \qquad x_0(t) := \int_0^t \gamma(s)ds. \tag{2}$$

Then, the system of equations (1) becomes

$$\dot{y} = e^{x_0(t)}N\left(e^{-x_0(t)}y\right). \tag{3}$$

Notice the same system of equations is achieved by multiplying (1) through by the integrating factor. In this way, a method for solving (1) can be constructed through standard methods that might be applied to (3), and the resulting methods are typically called integrating factor methods. More specifically, applying an RK method to (3) gives

$$\begin{aligned} Y_i &= y_n + h\sum_{j=1}^{s} \alpha_{ij} e^{x_0(t_n+c_jh)} N\left(e^{-x_0(t_n+c_jh)}Y_j\right), \quad i = 1, \dots, s, \\ y_{n+1} &= y_n + h\sum_{i=1}^{s} \beta_i e^{x_0(t_n+c_ih)} N\left(e^{-x_0(t_n+c_ih)}Y_i\right), \end{aligned}$$

where s is the number of stages, h denotes the step size, and $t_n = nh$ for $n = 0, 1, 2, \dots$. To write this in terms of the original variables, notice that

$$\int_{t_n+c_ih}^{t_n+h} \gamma(s)ds = \int_{t_n}^{t_n+h} \gamma(s)ds - \int_{t_n}^{t_n+c_ih} \gamma(s)ds = x_n(h) - x_n(c_ih),$$

where we define

$$x_n(t) = \int_0^t \gamma_n(s)ds \qquad \text{with} \qquad \gamma_n(s) := \gamma(s + t_n). \tag{4}$$

Thus, after manipulating the exponentials, the discretization can be rewritten in terms of the original variables to give a class of ERK methods for solving (1), which are often called IFRK methods, given by

$$
\begin{aligned}
Z_i &= e^{-x_n(c_i h)} z_n + h \sum_{j=1}^{s} \alpha_{ij} e^{x_n(c_j h) - x_n(c_i h)} N(Z_j), \quad i = 1, \dots, s, \\
z_{n+1} &= e^{-x_n(h)} z_n + h \sum_{i=1}^{s} \beta_i e^{-x_n(h) + x_n(c_i h)} N(Z_i),
\end{aligned} \tag{5}
$$

where $z_n \approx z(t_n)$ is the numerical solution.

A common alternative approach for constructing ERK methods is known as exponential time differencing, leading to the so-called ETDRK methods. To construct methods of this type, we use the variation of constants formula and write the solution of (1) as

$$
z(t) = e^{-x_0(t)} z(0) + e^{-x_0(t)} \int_0^t e^{x_0(\tau)} N(z(\tau)) d\tau,
$$

where $x_0(t)$ is defined in (2). Following [13], the integral here can be approximated using a polynomial interpolation of N, particularly when γ is constant. In cases where γ is truly time-dependent, we may also require an approximation of the integral defined by $x_n(t)$. A simple and likely approach, which is rooted in the work of Hipp, Hochbruck, and Ostermann [12], is to use an approximation, such as $x_n(h) \approx h\gamma_n(h/2)$.

In general, an s-stage ERK method for solving (1), which includes both IFRK and ETDRK formulations, can be stated as

$$
\begin{aligned}
Z_i &= \varphi_i(h; \gamma_n) z_n + h \sum_{j=1}^{s} a_{ij}(h; \gamma_n) N(Z_j), \quad i = 1, \dots, s, \\
z_{n+1} &= \varphi_0(h; \gamma_n) z_n + h \sum_{i=1}^{s} b_i(h; \gamma_n) N(Z_i).
\end{aligned} \tag{6}
$$

The *coefficients*, $\varphi_i, \varphi_0, a_{ij}$, and b_i, are scalar functions of the constant step size h, which also depend on the damping coefficient γ and the time step n, and they satisfy

$$
\varphi_i(h; 0) = \varphi_0(h; 0) = 1, \qquad a_{ij}(h; 0) = \alpha_{ij}, \qquad b_i(h; 0) = \beta_i \tag{7}
$$

for all $i, j = 1, 2, \dots, s$. The coefficients φ_i and φ_0 are either exponential functions or rational approximations of such functions. Here and throughout this paper we assume, for all i,

$$
\sum_{j=1}^{s} \alpha_{ij} = c_i \quad \text{and} \quad \sum_{i=1}^{s} \beta_i = 1. \tag{8}
$$

The RK method with coefficients α_{ij}, β_i is obtained from the ERK method by setting $\gamma = 0$ and is often referred to as the *underlying RK method*. An ERK method can be succinctly represented by a Butcher-like tableau, given by

$$
\begin{array}{c|c|c}
c & A & \varphi \\
\hline
 & b^T & \varphi_0
\end{array}. \tag{9}
$$

Entries c, φ, and b of the tableau are column vectors and A is a square matrix, such that

$$c = \{c_i\}_{i=1}^s, \qquad \varphi = \{\varphi_i\}_{i=1}^s, \qquad b = \{b_i\}_{i=1}^s, \qquad A = \{a_{ij}\}_{i,j=1}^s.$$

Since our focus is on structure preservation, natural choices for the underlying RK method are the Gauss–Legendre collocation methods, which are known to have order of accuracy $2s$, and symmetric methods [1] which satisfy the conditions

$$c_i = 1 - c_{s+1-i}, \qquad \beta_j = \alpha_{i,j} + \alpha_{s+1-i,s+1-j}, \qquad \beta_j = \beta_{s+1-j}$$

for all i, j. Examples of some importance in the following exposition are listed here.

- A second-order IFRK method based on the implicit midpoint rule (cf. [2])

$$\begin{array}{c|c|c} \frac{1}{2} & \frac{1}{2} & e^{-\int_{t_n}^{t_{n+1/2}} \gamma(s)ds} \\ \hline & e^{-\int_{t_{n+1/2}}^{t_{n+1}} \gamma(s)ds} & e^{-\int_{t_n}^{t_{n+1}} \gamma(s)ds} \end{array}. \tag{10}$$

- A second-order ETDRK method (with constant γ) based on the implicit midpoint rule

$$\begin{array}{c|c|c} \frac{1}{2} & \frac{1}{2\gamma h}(e^{\gamma h/2} - e^{-\gamma h/2}) & e^{-\gamma h/2} \\ \hline & \frac{1}{\gamma h}(1 - e^{-\gamma h}) & e^{-\gamma h} \end{array}. \tag{11}$$

- A fourth-order, two-stage, IFRK method (with constant γ)

$$\begin{array}{c|cc|c} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right) e^{\frac{\sqrt{3}}{3}\gamma h} & e^{-\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)\gamma h} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right) e^{-\frac{\sqrt{3}}{3}\gamma h} & \frac{1}{4} & e^{-\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)\gamma h} \\ \hline & \frac{1}{2} e^{-\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)\gamma h} & \frac{1}{2} e^{-\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)\gamma h} & e^{-\gamma h} \end{array}. \tag{12}$$

Other higher-order ERK methods can be constructed using the formulation (6).

Now, suppose the system of equations that is under consideration has the form

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} F(q,p) \\ G(q,p) \end{bmatrix} - \begin{bmatrix} \gamma^1(t) q \\ \gamma^2(t) p \end{bmatrix}, \quad \begin{bmatrix} q(0) \\ p(0) \end{bmatrix} = \begin{bmatrix} q_0 \\ p_0 \end{bmatrix}, \tag{13}$$

where $q, p \in \mathbb{R}^{d/2}$ with d even, and the functions $F, G : \mathbb{R}^d \to \mathbb{R}^{d/2}$ and $\gamma^k : \mathbb{R} \to \mathbb{R}$ for $k = 1, 2$ are smooth. We have suppressed the dependence of the variables q, p on t. To solve this system it may be desirable to employ one ERK method for the first equation and a different ERK method for the second. This approach yields a PERK method of the form

$$\begin{aligned} Q_i &= \widehat{\varphi}_i(h;\gamma_n^1) q_n + h \sum_{j=1}^s \widehat{a}_{ij}(h;\gamma_n^1) F(Q_j, P_j), \quad i = 1, \dots, s, \\ P_i &= \widetilde{\varphi}_i(h;\gamma_n^2) p_n + h \sum_{j=1}^s \widetilde{a}_{ij}(h;\gamma_n^2) G(Q_j, P_j), \quad i = 1, \dots, s, \\ q_{n+1} &= \widehat{\varphi}_0(h;\gamma_n^1) q_n + h \sum_{i=1}^s \widehat{b}_i(h;\gamma_n^1) F(Q_i, P_i), \\ p_{n+1} &= \widetilde{\varphi}_0(h;\gamma_n^2) p_n + h \sum_{i=1}^s \widetilde{b}_i(h;\gamma_n^2) G(Q_i, P_i), \end{aligned} \tag{14}$$

where *coefficients*, $\widehat{\varphi}_0, \widehat{\varphi}_i, \widehat{a}_{ij}, \widehat{b}_j, \widetilde{\varphi}_0, \widetilde{\varphi}_i, \widetilde{a}_{ij},$ and $\widetilde{b}_j$ are scalar functions and they must satisfy the conditions required of an ERK method, namely, (7) and (8). Here, Q_i, P_i are stage variables, $[q_n, p_n] \approx [q(t_n), p(t_n)]$ is the numerical solution for $n = 0, 1, 2, \ldots$ and $t_n = nh$, and γ_n^k for $k = 1, 2$ are defined according to (4). In this case, the *underlying method* is a PRK method, obtained by setting $\gamma^k = 0$ for $k = 1, 2$. (For our purposes, the Lobatto IIIA-IIIB methods are natural choices for the underlying PRK methods.) A PERK method can be succinctly represented by a pair of Butcher-like tableau, given by

$$\text{(15)} \qquad \begin{array}{c|c|c} \widehat{c} & \widehat{A} & \widehat{\varphi} \\ \hline \widehat{\ } & \widehat{b}^T & \widehat{\varphi}_0 \end{array}, \qquad \begin{array}{c|c|c} \widetilde{c} & \widetilde{A} & \widetilde{\varphi} \\ \hline \widetilde{\ } & \widetilde{b}^T & \widetilde{\varphi}_0 \end{array},$$

one for each ERK method used. Notice that setting

$$\widehat{\varphi}_0 = \widetilde{\varphi}_0 = \varphi_0, \quad \widehat{\varphi}_i = \widetilde{\varphi}_i = \varphi_i, \quad \widehat{a}_{ij} = \widetilde{a}_{ij} = a_{ij}, \quad \widehat{b}_j = \widetilde{b}_j = b_j \quad \text{for all } i, j$$

in a PERK method gives an ERK method.

As an example, consider an important special case of the ODE system (13), given by

$$\dot{q} = \nabla_p T(p), \qquad \dot{p} = -\nabla_q V(q) - \gamma p,$$

with $0 < \gamma \in \mathbb{R}$, which is known as a conformal Hamiltonian system [19]. If one or both equations of this system are discretized with an IFRK or ETDRK method, we refer to such a PERK method as an *IFPRK* or an *ETDPRK* method, respectively. Some examples of PERK methods for solving the system are

- a first-order IFPRK method based on the symplectic Euler method

$$\text{(16)} \qquad q_{n+1} = q_n + h\nabla_p T(p_{n+1}), \qquad p_{n+1} = e^{-\gamma h} p_n - h\nabla_q V(q_n),$$

- a first-order ETDPRK method based on the symplectic Euler method

$$\text{(17)} \quad q_{n+1} = q_n + h\nabla_p T(p_{n+1}), \qquad p_{n+1} = e^{-\gamma h} p_n + \frac{1}{\gamma}(e^{-\gamma h} - 1)\nabla_q V(q_n),$$

- a second-order IFPRK method based on the two-stage Lobatto IIIA-IIIB (Störmer–Verlet) method

$$\text{(18)} \qquad \begin{array}{c|cc|c} 0 & 0 & 0 & 1 \\ 1 & \frac{1}{2} & \frac{1}{2} & 1 \\ \hline \widehat{\ } & \frac{1}{2} & \frac{1}{2} & 1 \end{array}, \qquad \begin{array}{c|cc|c} \frac{1}{2} & \frac{1}{2} & 0 & e^{-\gamma h/2} \\ \frac{1}{2} & \frac{1}{2} & 0 & e^{-\gamma h/2} \\ \hline \widetilde{\ } & \frac{1}{2}e^{-\gamma h/2} & \frac{1}{2}e^{-\gamma h/2} & e^{-\gamma h} \end{array},$$

- a second-order IFPRK method based on the two-stage Lobatto IIIA-IIIB method

$$\text{(19)} \qquad \begin{array}{c|cc|c} 0 & 0 & 0 & 1 \\ \frac{4}{4-\gamma h} & \frac{2}{4-\gamma h} & \frac{2}{4-\gamma h} & \frac{4+\gamma h}{4-\gamma h}e^{-\gamma h/2} \\ \hline \widehat{\ } & \frac{2}{4-\gamma h} & \frac{2}{4-\gamma h} & \frac{4+\gamma h}{4-\gamma h}e^{-\gamma h/2} \end{array}, \qquad \begin{array}{c|cc|c} \frac{2}{4+\gamma h} & \frac{2}{4+\gamma h} & 0 & \frac{4}{4+\gamma h}e^{-\gamma h/4} \\ \frac{2}{4+\gamma h} & \frac{2}{4+\gamma h} & 0 & \frac{4}{4+\gamma h}e^{-\gamma h/4} \\ \hline \widetilde{\ } & \frac{4-\gamma h}{4+\gamma h}\frac{e^{-\gamma h/4}}{2} & \frac{e^{-\gamma h/4}}{2} & \frac{4-\gamma h}{4+\gamma h}e^{-\gamma h/2} \end{array},$$

- a second-order ETDPRK method based on the two-stage Lobatto IIIA-IIIB method

$$(20)\quad \begin{array}{c|cc|c} 0 & 0 & 0 & 1 \\ 1 & \frac{1}{2} & \frac{1}{2} & 1 \\ \hline \widehat{\ } & \frac{1}{2} & \frac{1}{2} & 1 \end{array}, \qquad \begin{array}{c|cc|c} \frac{1}{2} & \frac{1}{\gamma h}(1-e^{-\gamma h/2}) & 0 & e^{-\gamma h/2} \\ \frac{1}{2} & \frac{1}{\gamma h}(1-e^{-\gamma h/2}) & 0 & e^{-\gamma h/2} \\ \hline \sim & \frac{1}{2}e^{-\gamma h/2} & \frac{1}{2}e^{-\gamma h/2} & e^{-\gamma h} \end{array}.$$

Methods (18) and (19) have been analyzed in some detail in [2, 24], where one can find applications to ODEs and PDEs, in addition to linear stability analysis and structure-preservation properties for conformal Hamiltonian systems.

Though this discussion has been somewhat limited to integrating factor methods and exponential time differencing methods, other exponential integrators may be included in the general ERK and PERK formulations given in (6) and (14). It is important to keep this in mind, as the proofs concerning structure preservation for ERK and PERK methods in the following sections give restrictions on the coefficient functions, which include, but are not necessarily limited to, integrating factor and exponential time differencing methods.

3. Preservation of conformal invariants. This section is devoted to deriving sufficient conditions for preservation of conformal invariants by ERK and PERK methods. Some of the methods of the previous section are shown to satisfy these conditions.

DEFINITION 3.1. *A nonconstant function* $\mathcal{I}(t) : \mathbb{R}^d \to \mathbb{R}$ *is a* conformal invariant *of* (1) *if*

$$\frac{d}{dt}\mathcal{I} = -2\gamma(t)\mathcal{I}, \tag{21}$$

where $\gamma(t) : \mathbb{R} \to \mathbb{R}$ *and* $\mathcal{I}$ *is a function of the solution* $z(t)$*. Similarly, a nonconstant function* $\mathcal{I}(t) : \mathbb{R}^{2d} \to \mathbb{R}$ *is a* conformal invariant *of* (13) *if*

$$\frac{d}{dt}\mathcal{I} = -(\gamma^1(t) + \gamma^2(t))\mathcal{I},$$

where $\mathcal{I}$ *is a function of* q *and* p*.*

Notice that (21) is equivalent to

$$\frac{d}{dt}\left(e^{\int_0^t 2\gamma(s)ds}\mathcal{I}(t)\right) = 0 \qquad \Longleftrightarrow \qquad \mathcal{I}(t) = e^{-\int_0^t 2\gamma(s)ds}\mathcal{I}(0).$$

Some examples of equations and their respective conformal invariants are given in Table 1. These equations can be put in the form (1) using suitable discretizations of any spatial derivative(s). It is straightforward to show that the quantities in the second column of the table satisfy (21) along solutions of the corresponding differential equation.

Conformal invariants precisely describe the effects of a nonconservative perturbation on the dynamics. For example, in the case of constant (but small) $\gamma > 0$, formula (21) embodies the dissipation of some quantity, such as the energy or the symplectic form, which is intimately connected to the solution behavior. Some numerical methods "preserve" dissipative properties by simply guaranteeing that $\mathcal{I}$ is decreasing with every time step, even though it the may be numerically overdamped or underdamped. Thus, it is natural to expect that numerical methods which exactly

TABLE 1
Some equations and their conformal invariants, under suitable boundary conditions where applicable. In every equation, setting $\gamma = 0$ gives the conservative counterpart of the equation.

Equation	Conformal invariant
Damped harmonic oscillator $q_{tt} + 2\gamma q_t + \kappa^2 q = 0$	$\mathcal{I} = \frac{1}{2}(\kappa^2 q^2 + q_t^2) + \gamma q q_t$
Damped nonlinear Schrödinger equation $\mathtt{i}\psi_t + \psi_{xx} + V'(\lvert\psi\rvert^2)\psi + \mathtt{i}\gamma\psi = 0$	$\mathcal{I} = \int \lvert\psi\rvert^2 \, dx$
Damped Camassa Holm equation $u_t - u_{xxt} + 3uu_x + \gamma(u - u_{xx}) = 2u_x u_{xx} + uu_{xxx}$	$\mathcal{I} = \int (u^2 + u_x^2) \, dx$
Damped wave equation $u_{tt} - u_{xx} + cu + 2\gamma u_t = 0$	$\mathcal{I} = \int u_t u_x \, dx$
Damped KdV equation $u_t + uu_x + u_{xxx} + 2\gamma u = 0$	$\mathcal{I} = \int u \, dx$

preserve conformal invariants have certain advantages other methods, and the special form of (21) leads to a simple and straightforward definition of a method that exactly preserves a conformal invariant.

DEFINITION 3.2. *A numerical method* $z_{n+1} = \Psi_h(z_n)$ preserves *a conformal invariant* $\mathcal{I}$ *of* (1) *if it satisfies*

$$\mathcal{I}_{n+1} = e^{-\int_{t_n}^{t_{n+1}} 2\gamma(s)ds} \mathcal{I}_n,$$

where $\mathcal{I}_n = \mathcal{I}(t_n)$ *(cf.* [2]*). Similarly, a numerical method* $z_{n+1} = \Psi_h(z_n)$ preserves *a conformal invariant* $\mathcal{I}$ *of* (13) *if it satisfies*

$$\mathcal{I}_{n+1} = e^{-\int_{t_n}^{t_{n+1}} (\gamma^1(s) + \gamma^2(s))ds} \mathcal{I}_n,$$

where $\mathcal{I}_n = \mathcal{I}(t_n)$.

In the following, we derive sufficient conditions for structure preservation by PERK methods in line with similar conditions for PRK methods.

THEOREM 3.3. *Suppose that the system* (13) *has a conformal invariant* $\mathcal{I} = q^T W p$*, with a constant matrix* $W \in \mathbb{R}^{d/2 \times d/2}$*. Then a PERK method applied to such a system satisfies* $\mathcal{I}_{n+1} = \widehat{\varphi}_0 \widetilde{\varphi}_0 \mathcal{I}_n$*, provided its coefficients satisfy*

$$\widehat{b}_i \frac{\widetilde{\varphi}_0}{\widetilde{\varphi}_i} = \widetilde{b}_i \frac{\widehat{\varphi}_0}{\widehat{\varphi}_i}, \qquad \widehat{b}_i \widetilde{a}_{ij} \frac{\widetilde{\varphi}_0}{\widetilde{\varphi}_i} + \widetilde{b}_j \widehat{a}_{ji} \frac{\widehat{\varphi}_0}{\widehat{\varphi}_j} - \widehat{b}_i \widetilde{b}_j = 0 \tag{22}$$

for all i, j.

Proof. Using the Kronecker product $\otimes$, one can write the system (14) as

$$\begin{aligned} Q &= \widehat{\varphi} \otimes q_n + h(\widehat{A} \otimes I)F, \\ P &= \widetilde{\varphi} \otimes p_n + h(\widetilde{A} \otimes I)G, \\ q_{n+1} &= \widehat{\varphi}_0 q_n + h(\widehat{b}^T \otimes I)F, \\ p_{n+1} &= \widetilde{\varphi}_0 p_n + h(\widetilde{b}^T \otimes I)G, \end{aligned} \tag{23}$$

where $I \in \mathbb{R}^{d/2 \times d/2}$ is the identity matrix, and we define the vectors $Q = \{Q_i\}_{i=1}^s$, $P = \{P_i\}_{i=1}^s$, $F = \{F_i\}_{i=1}^s$, and $G = \{G_i\}_{i=1}^s$, with $F_i = F(Q_i, P_i)$ and $G_i = G(Q_i, P_i)$.

This implies that

$$q_{n+1}^T W p_{n+1} = \widehat{\varphi}_0\widetilde{\varphi}_0 q_n^T W p_n + h\widehat{\varphi}_0 q_n^T W(\widetilde{b}^T \otimes I)G + h\widetilde{\varphi}_0((\widehat{b}^T \otimes I)F)^T W p_n + h^2((\widehat{b}^T \otimes I)F)^T W(\widetilde{b}^T \otimes I)G,$$

which is equivalent to

$$q_{n+1}^T W p_{n+1} = \widehat{\varphi}_0\widetilde{\varphi}_0 q_n^T W p_n + h\widehat{\varphi}_0 q_n^T(\widetilde{b}^T \otimes W)G + h\widetilde{\varphi}_0 F^T(\widehat{b} \otimes W)p_n + h^2 F^T(\widehat{b}\widetilde{b}^T \otimes W)G. \tag{24}$$

Let $\widetilde{B}, \widehat{B} \in \mathbb{R}^{s\times s}$ be diagonal matrices such that

$$\widetilde{B}\widetilde{\varphi} = \widetilde{b} \qquad \text{and} \qquad \widehat{B}\widetilde{\varphi} = \widehat{b}, \tag{25}$$

respectively. Then using (23) once again

$$Q^T(\widetilde{B} \otimes W)G = (\widehat{\varphi}^T \otimes q_n^T)(\widetilde{B} \otimes W)G + hF^T(\widehat{A}^T \otimes I)(\widetilde{B} \otimes W)G = q_n^T(\widetilde{b}^T \otimes W)G + hF^T(\widehat{A}^T\widetilde{B} \otimes W)G \tag{26}$$

and

$$F^T(\widehat{B} \otimes W)P = F^T(\widehat{b}^T \otimes W)p_n + hF^T(\widehat{B}\widetilde{A} \otimes W)G. \tag{27}$$

Using (26)–(27) in (24), one gets

$$q_{n+1}^T W p_{n+1} = \widehat{\varphi}_0\widetilde{\varphi}_0 q_n^T W p_n + h\widehat{\varphi}_0 Q^T(\widetilde{B} \otimes W)G + h\widetilde{\varphi}_0 F^T(\widehat{B} \otimes W)P + h^2 F^T((\widehat{\widetilde{b}\widetilde{b}}^T - \widehat{\varphi}_0\widehat{A}^T\widetilde{B} - \widetilde{\varphi}_0\widehat{B}\widetilde{A}) \otimes W)G. \tag{28}$$

On the other hand, since $\mathcal{I}$ is a conformal invariant, it follows that

$$0 = q^T W G(q,p) + F(q,p)^T W p$$

for all q, p. Thus, provided $\widehat{b}_i\frac{\widetilde{\varphi}_0}{\widetilde{\varphi}_i} = \widetilde{b}_i\frac{\widehat{\varphi}_0}{\widehat{\varphi}_i}$ for all i,

$$0 = Q_i^T W G_i + F_i^T W P_i = Q_i^T\widetilde{b}_i\frac{\widehat{\varphi}_0}{\widehat{\varphi}_i}WG_i + F_i^T\widehat{b}_i\frac{\widetilde{\varphi}_0}{\widetilde{\varphi}_i}WP_i,$$

which implies

$$0 = \sum_{i=1}^{s} Q_i^T\widetilde{b}_i\frac{\widehat{\varphi}_0}{\widehat{\varphi}_i}WG_i + F_i^T\widehat{b}_i\frac{\widetilde{\varphi}_0}{\widetilde{\varphi}_i}WP_i = \widehat{\varphi}_0 Q^T(\widetilde{B} \otimes W)G + \widetilde{\varphi}_0 F^T(\widehat{B} \otimes W)P.$$

Using this and (22) in (28), we get

$$q_{n+1}^T W p_{n+1} = \widehat{\varphi}_0\widetilde{\varphi}_0 q_n^T W p_n. \qquad \square$$

The following corollary is a consequence of Theorem 3.3 and Definition 3.2.

COROLLARY 3.4. *If in addition to the hypotheses of Theorem* 3.3*, a PERK method also satisfies*

$$\widehat{\varphi}_0\widetilde{\varphi}_0 = e^{-\int_{t_n}^{t_{n+1}}(\gamma^1(s)+\gamma^2(s))ds},$$

then it preserves the conformal invariant $\mathcal{I}$*.*

For example, the conformal invariant of damped harmonic oscillator in Table 1 is a quadratic conformal invariant because

$$\begin{aligned}\mathcal{I} &= \tfrac{1}{2}(\kappa^2 q^2 + q_t^2) + \gamma q q_t \\ &= \begin{bmatrix} q & q_t \end{bmatrix} \begin{bmatrix} \frac{1}{2}\kappa^2 & \frac{1}{2}\gamma \\ \frac{1}{2}\gamma & \frac{1}{2} \end{bmatrix} \begin{bmatrix} q \\ q_t \end{bmatrix}.\end{aligned}$$

Semidiscretizing a PDE in space, one can approximate some of the conformal invariants for PDEs in Table 1 by quadratic conformal invariants, e.g.,

$$\mathcal{I} = \int |\psi|^2 \, dx \approx \sum \psi_n \cdot \psi_n^* \, \Delta x,$$

where $\psi_n = \{\psi_{n,i}\}_{i=1}^M$ is the numerical solution vector at the temporal index n and $*$ denotes the complex conjugate. Here i is the spatial index. Some of the other conformal invariants for PDEs in the table can be similarly approximated by quadratic and linear conformal invariant. Among the PERK methods (16)–(20) introduced in the previous section, only methods (16) and (18) satisfy the hypotheses of Corollary 3.4, and hence for these methods,

$$q_{n+1}^T W p_{n+1} = e^{-\gamma h}(q_n^T W p_n),$$

i.e., they preserve the conformal quadratic invariant $q^T W p$.

THEOREM 3.5. *Let the function $\mathcal{I} = \sigma_1^T q + \sigma_2^T p$, with constant vectors $\sigma_1, \sigma_2 \in \mathbb{R}^{d/2}$, be a conformal invariant of the system* (13)*, and assume one of the following three conditions is satisfied:* (i) $\gamma^1(t) = \gamma^2(t) = \gamma(t)$, (ii) $\sigma_1 = 0$, *or* (iii) $\sigma_2 = 0$. *Then, a PERK method for such a system satisfies*

$$\sigma_1^T q_{n+1} + \sigma_2^T p_{n+1} = \widehat{\varphi}_0 \sigma_1^T q_n + \widetilde{\varphi}_0 \sigma_2^T p_n,$$

provided its coefficients satisfy $\widetilde{b}_i = \widehat{b}_i$.

Proof. Formulation (23) of the PERK method implies

$$\sigma_1^T q_{n+1} + \sigma_2^T p_{n+1} = \widehat{\varphi}_0 \sigma_1^T q_n + \widetilde{\varphi}_0 \sigma_2^T p_n + \sigma_1^T (\widehat{b}^T \otimes I) F + \sigma_2^T (\widetilde{b}^T \otimes I) G.$$

Thus, to obtain the desired result, we must show that

$$\sigma_1^T (\widehat{b}^T \otimes I) F + \sigma_2^T (\widetilde{b}^T \otimes I) G = 0.$$

But, this follows from the fact that

$$0 = \sigma_1^T F_i + \sigma_2^T G_i = \sigma_1^T \widehat{b}_i F_i + \sigma_2^T \widetilde{b}_i G_i = \sum_{i=1}^{s} \sigma_1^T \widehat{b}_i F_i + \sigma_2^T \widetilde{b}_i G_i,$$

because $\mathcal{I}$ is a conformal invariant of the system (13) with $\gamma^1(t) = \gamma^2(t) = \gamma(t)$, meaning $\sigma_1^T F(q,p) + \sigma_2^T G(q,p) = 0$ for all q, p. The result for cases (ii) and (iii) follows automatically. ∎

COROLLARY 3.6. *If in addition to the hypotheses of Theorem* 3.5*, a PERK method also satisfies*

$$\widehat{\varphi}_0 = e^{-\int_{t_n}^{t_{n+1}} \gamma^1(s) ds}, \; \widetilde{\varphi}_0 = e^{-\int_{t_n}^{t_{n+1}} \gamma^2(s) ds},$$

then the method preserves the conformal invariant $\mathcal{I}$.

Among the PERK methods (16)–(20) introduced in the previous section, only method (16) satisfies the hypotheses of this corollary and preserves the conformal linear invariants $\sigma_1^T q + \sigma_2^T p$.

The following result about the structure-preserving properties of the ERK method can be derived in a manner analogous to those of the PERK method.

THEOREM 3.7. *Suppose the system* (1) *has a conformal invariant* $\mathcal{I} = z^T W z$ *where* $W \in \mathbb{R}^{d\times d}$ *is a constant symmetric matrix. Then an ERK method applied to such a system satisfies* $\mathcal{I}_{n+1} = \varphi_0^2 \mathcal{I}_n$ *provided its coefficients satisfy*

$$b_i a_{ij} \frac{\varphi_0}{\varphi_i} + b_j a_{ji} \frac{\varphi_0}{\varphi_j} - b_i b_j = 0 \tag{29}$$

for all i, j.

COROLLARY 3.8. *If in addition to the hypotheses of Theorem* 3.7*, an ERK method also satisfies*

$$\varphi_0 = e^{-\int_{t_n}^{t_{n+1}} \gamma(s) ds}, \tag{30}$$

then the method preserves the conformal invariant $\mathcal{I}$.

The methods defined by (10)–(12) all satisfy the hypotheses of this corollary, and hence they have the property

$$z_{n+1}^T W z_{n+1} = e^{-2\gamma h} z_n^T W z_n,$$

i.e., these methods preserve conformal invariants of the form $z^T W z$. The following theorem follows directly from the definition of ERK methods.

THEOREM 3.9. *Suppose that the system* (1) *has a conformal invariant* $\mathcal{I} = \sigma^T z$*, with constant vector* $\sigma \in \mathbb{R}^d$*. Then an ERK method applied to such a system satisfies* $\mathcal{I}_{n+1} = \varphi_0 \mathcal{I}_n$.

COROLLARY 3.10. *If in addition to the hypotheses of Theorem* 3.9*, an ERK method also satisfies* (30)*, then the method preserves the conformal invariant* $\mathcal{I}$.

Since all the methods (10)–(12) satisfy the hypotheses of this corollary, all these methods preserve conformal linear invariants.

4. Preservation of conformal symplecticity. In this section, we derive conformal symplecticity conditions for the ERK and the PERK methods. Substituting $N(z) = \mathbf{J}^{-1} \nabla_z H(z)$ in (1), we get the conformal Hamiltonian system [19]

$$\dot{z} = \mathbf{J}^{-1} \nabla_z H(z) - \gamma(t) z, \tag{31}$$

where

$$z = \begin{bmatrix} q \\ p \end{bmatrix} \quad \text{and} \quad \mathbf{J}^{-1} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$$

is a constant skew-symmetric matrix. Here $I \in \mathbb{R}^{d/2\times d/2}$ is the identity matrix. From the variational equation associated with (31)

$$d\dot{z} = \mathbf{J}^{-1} H_{zz}(z) dz - \gamma(t) dz, \tag{32}$$

where $H_{zz}(z)$ is the Hessian matrix, one can easily obtain $\dot{\omega} = -2\gamma(t)\omega$, where $\omega = dz \wedge \mathbf{J} dz$, assuming $H_{zz}(z)$ is symmetric.

Substituting $F = \nabla_p \mathcal{H}(q,p)$, $G = -\nabla_q \mathcal{H}(q,p)$, along with $\gamma^1 = 0$ and $\gamma^2 = \gamma$ in (13), we get

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} \nabla_p \mathcal{H}(q,p) \\ -\nabla_q \mathcal{H}(q,p) \end{bmatrix} - \begin{bmatrix} 0 \\ \gamma(t)p \end{bmatrix}, \qquad \begin{bmatrix} q(0) \\ p(0) \end{bmatrix} = \begin{bmatrix} q_0 \\ p_0 \end{bmatrix}. \tag{33}$$

From this equation, one can obtain

$$\dot{\omega} = -\gamma(t)\omega$$

for $\omega = dq \wedge dp$. Thus, we arrive at the following definitions.

DEFINITION 4.1. *Differential equations* (1) *and* (13) *are called* conformal symplectic *if the differential two-forms*

$$\omega = dz \wedge \mathbf{J} dz \text{ and } \omega = dq \wedge dp,$$

respectively, are conformal invariants of the corresponding equations.

DEFINITION 4.2. *A numerical method* $z_{n+1} = \Psi_h(z_n)$ *for solving differential equations* (1) *and* (13) *is said to* preserve conformal symplecticity*, and we call such a method conformal symplectic, if it preserves the corresponding conformal invariants of Definition* 4.1.

Please refer to Definitions 3.1 and 3.2 for the definitions of conformal invariants of a differential equation and their preservation by a numerical method. The following theorems concerning conformal symplecticity of the PERK and ERK methods adopt the proof strategy presented in [17] for Hamiltonian systems.

THEOREM 4.3. *A PERK method for* (33) *satisfies*

$$dq_{n+1} \wedge dp_{n+1} = \widehat{\varphi}_0 \widetilde{\varphi}_0 \, (dq_n \wedge dp_n)$$

provided its coefficients satisfy (22).

Proof. The variational equation associated with the PERK method (23) applied to system (33) is

$$\begin{aligned} dQ &= \widehat{\varphi} \otimes dq_n + h(\widehat{A} \otimes I) dF, \\ dP &= \widetilde{\varphi} \otimes dp_n + h(\widetilde{A} \otimes I) dG, \\ dq_{n+1} &= \widehat{\varphi}_0 dq_n + h(\widehat{b}^T \otimes I) dF, \\ dp_{n+1} &= \widetilde{\varphi}_0 dp_n + h(\widetilde{b}^T \otimes I) dG, \end{aligned} \tag{34}$$

where $F_i = \nabla_p \mathcal{H}(Q_i, P_i)$, $G_i = -\nabla_q \mathcal{H}(Q_i, P_i)$, $dF = F_Q dQ + F_P dP$, and $dG = G_Q dQ + G_P dP$. This implies that

$$\partial_{Q_i} F_i + \partial_{P_i} G_i = \nabla_{pq} \mathcal{H}(Q_i, P_i) - \nabla_{qp} \mathcal{H}(Q_i, P_i) = 0 \quad \text{for all } i,$$

and hence $F_Q^T + G_P = 0$. Also $F_P = F_P^T$ and $G_Q = G_Q^T$. Now, system (34) implies

$$\begin{aligned} &dq_{n+1} \wedge dp_{n+1} - \widehat{\varphi}_0 \widetilde{\varphi}_0 dq_n \wedge dp_n \\ &\quad = h \widehat{\varphi}_0 dq_n \wedge (\widetilde{b}^T \otimes I) dG - h \widetilde{\varphi}_0 dp_n \wedge (\widehat{b}^T \otimes I) dF + h^2 dF \wedge (\widehat{b}\widetilde{b}^T \otimes I) dG. \end{aligned} \tag{35}$$

Using the first and second equations of the system (34) and letting $\widetilde{B}$ and $\widehat{B}$ be diagonal matrices such that they satisfy (25), we get

$$\begin{aligned} dQ \wedge (\widetilde{B} \otimes I)dG &= \widehat{\varphi} \otimes dq_n \wedge (\widetilde{B} \otimes I)dG + h(\widehat{A} \otimes I)dF \wedge (\widetilde{B} \otimes I)dG \\ &= dq_n \wedge (\widetilde{b}^T \otimes I)dG + hdF \wedge (\widehat{A}^T \widetilde{B} \otimes I)dG \end{aligned} \tag{36}$$

and

$$dP \wedge (\widehat{B} \otimes I)dF = dp_n \wedge (\widehat{b}^T \otimes I)dF + hdG \wedge (\widetilde{A}^T \widehat{B} \otimes I)dF. \tag{37}$$

Using (36)–(37) in (35) we get

$$\begin{aligned} dq_{n+1} \wedge dp_{n+1} - \widehat{\varphi}_0 \widetilde{\varphi}_0 dq_n \wedge dp_n &= hdQ \wedge (\widetilde{B}\widehat{\varphi}_0 \otimes I)dG - hdP \wedge (\widehat{B}\widetilde{\varphi}_0 \otimes I)dF \\ &\quad - h^2 dF \wedge ((\widehat{\varphi}_0 \widehat{A}^T \widetilde{B} + \widetilde{\varphi}_0 \widehat{B}^T \widetilde{A} - \widetilde{\widehat{b}\widetilde{b}^T}) \otimes I)dG. \end{aligned} \tag{38}$$

Since $G_P + F_Q^T = 0$ and (22) implies $\widetilde{B}\widehat{\varphi}_0 = \widehat{B}\widetilde{\varphi}_0$, we have

$$dQ \wedge (\widetilde{B}\widehat{\varphi}_0 \otimes I)dG - dP \wedge (\widehat{B}\widetilde{\varphi}_0 \otimes I)dF = dQ \wedge (\widetilde{B}\widehat{\varphi}_0 \otimes I)(G_P + F_Q^T)dP = 0.$$

Using this and (22) in (38) yields the desired result. ∎

COROLLARY 4.4. *A PERK method for* (33) *is conformal symplectic if it satisfies the hypotheses of Theorem* 4.3 *and*

$$\widehat{\varphi}_0 \widetilde{\varphi}_0 = e^{-\int_{t_n}^{t_{n+1}} \gamma(s)ds}.$$

One can obtain a similar result for the ERK method.

THEOREM 4.5. *An ERK method for* (31) *satisfies*

$$dz_{n+1} \wedge \mathbf{J} dz_{n+1} = \varphi_0^2 \, (dz_n \wedge \mathbf{J} dz_n)$$

provided its coefficients satisfy (29).

COROLLARY 4.6. *An ERK method is conformal symplectic if it satisfies the hypotheses of Theorem* 4.5 *and* (30).

PERK methods (16) and (18) satisfy the hypotheses of Corollary 4.4 and ERK methods (10)–(12) satisfy the hypotheses of Corollary 4.6; hence, these methods are conformal symplectic. Although methods (17) and (19) do not satisfy the condition (22) it is a quick calculation to show that they are also conformal symplectic. Moreover (19) has a conformal quadratic invariance [2]. This shows that a PERK method does not necessarily need to satisfy the condition (22) in order to preserve these geometric properties. Method (20) neither satisfies the condition (22) nor is conformal symplectic, so it is not enough to use any ERK method which has a conservative underlying RK method. It is interesting to note that the conditions (22) and (29) are sufficient for both conformal quadratic invariance and conformal symplecticity of the respective methods (cf. [3]).

There are a few important implications of Corollaries 4.4 and 4.6. First, combining the hypotheses of the corollaries with the conditions (7) implies that the underlying RK and PRK methods are always symplectic. Additionally, if $\psi_t(z_0)$ is the flow map

of the system (31) at time t with initial condition z_0, then an alternative (equivalent) formulation of the conformal symplectic property given in Definition 4.1 is

$$(\psi_t'(z_0))^T \mathbf{J}^{-1} \psi_t'(z_0) = e^{-2\int_0^t \gamma(s)ds} \mathbf{J}^{-1}, \tag{39}$$

where $\psi_t'(z_0)$ denotes the Jacobian. This formula can be derived from the variational equation

$$\frac{d}{dt}[\psi_t'] = \mathbf{J}^{-1} H_{zz}(z)\psi_t' - \gamma(t)\psi_t'$$

by taking the time derivative of $(\psi_t'(z_0))^T \mathbf{J}^{-1} \psi_t'(z_0)$. Thus, if Ψ_h is the flow map of a conformal symplectic ERK method, then

$$(\Psi_h'(z_n))^T \mathbf{J}^{-1} (\Psi_h'(z_n)) = e^{-2\int_{t_n}^{t_{n+1}} \gamma(s)ds} \mathbf{J}^{-1}. \tag{40}$$

If the method is applied to the linear scalar ODE $z_t = (\gamma + \lambda)z$, then (40) implies

$$\det(\Psi_h'(z_n)) = |R(\lambda h, \gamma h)| = e^{-\gamma h},$$

where R is the stability function of the ERK method. This shows that the methods preserve the dissipative part of the flow for this simple linear equation. Furthermore, the stability function of a conformal symplectic ERK method may be written in the form $R(\lambda h, \gamma h) = e^{-\gamma h} r(\lambda h, \gamma h)$, where $|r(\lambda h, \gamma h)| = 1$ and $\lim_{\gamma \to 0} r(\lambda h, \gamma h) = R_0(\lambda h)$ is the stability function of the underlying RK method, since the underlying RK method is symplectic, and since an RK method is symplectic if, and only if, its stability function satisfies $|R_0(\lambda h)| = 1$ for all $\lambda > 0$ [10].

5. Numerical experiments. The second-order ERK and PERK methods given by (10), (18), and (19) have been applied to various ODEs and PDEs with constant damping coefficients to demonstrate their properties of structure preservation [2, 24]. Studies have also performed numerical simulations using various first-order ERK methods on very similar problems [14, 25, 26, 30]. Our purpose in this section is to demonstrate the effectiveness of ERK and PERK methods from a few points of view that are different from previous studies. First, we demonstrate preservation of conformal symplecticity. Second, we consider problems with time-dependent damping. Third, we conduct experiments using methods of higher orders (four and six). Fourth, we illustrate the advantages of such methods for a damped Poisson (noncanonical) system. Fifth, we implement structure-preserving exponential time differencing methods and compare the results to more commonly used integrating factor methods.

5.1. Damped oscillator. Consider the following linear ODE:

$$\ddot{q} + 2\gamma(t)\dot{q} + \kappa^2 q = 0, \tag{41}$$

where $\kappa \in \mathbb{R}$. We analyze numerical simulations in two cases: $\gamma = \text{const.}$ and $\gamma(t) = \frac{1}{2}\varepsilon \cos(2t)$ with $\varepsilon \in \mathbb{R}$.

5.1.1. Constant damping. To begin, we compare the integrating factor and exponential time differencing methods given in (16) and (17), respectively. Both methods are first order, and both are conformal symplectic. Figure 1 shows the average absolute error for each method, as γ is fixed, while the frequency and the step size are varied. Notice the exponential time differencing method exhibits clear advantages over the integrating factor method as the frequency increases, and these

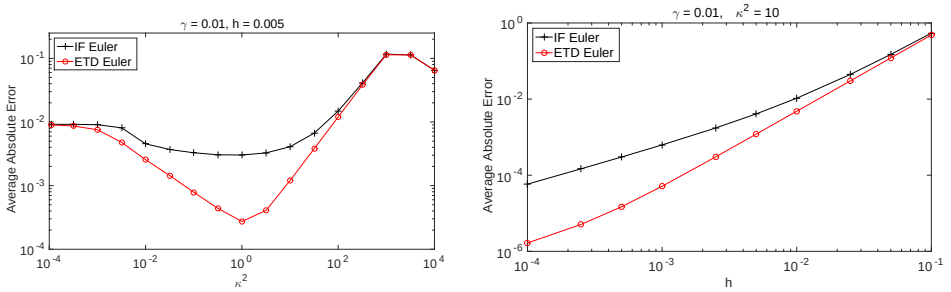

FIG. 1. *A comparison of the average absolute solution error for the conformal symplectic Euler methods given in* (16) *and* (17) *for solving* (41) *with* $\gamma = 0.01$. *Initial condition:* $q(0) = 0$, $\dot{q}(0) = 10$; *final time:* $T = 50$.

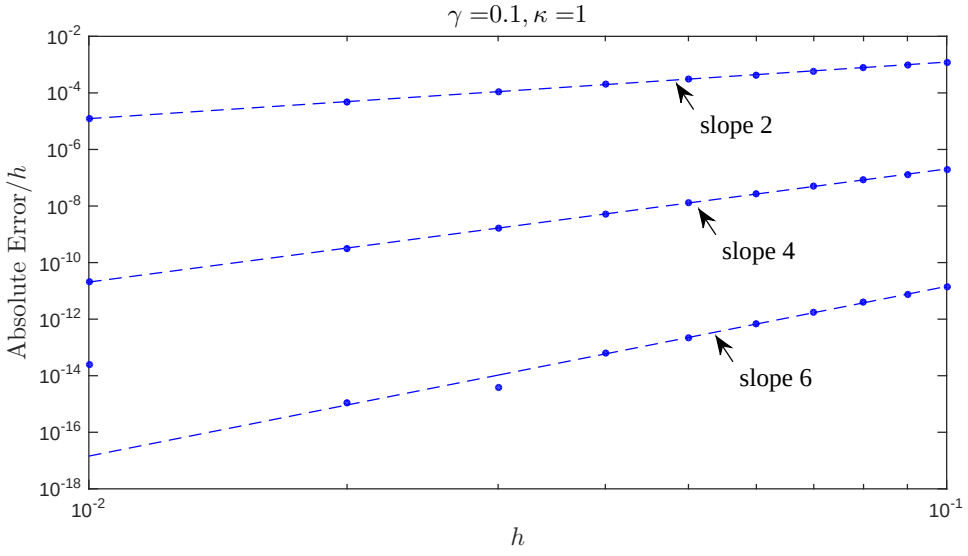

FIG. 2. *Local absolute error in solution over the step size for IFRK methods of stages* 1, 2, *and* 3 *applied to ODE* (41). *Dashed lines represent the slopes with which they are labeled.*

advantages are more pronounced as the step size decreases, even for problems with high frequencies.

Next, we present an example illustrating order of accuracy and structure preservation by IFRK methods, which have the Gauss–Legendre schemes as the underlying RK methods. For the sake of convenience we call them GL-IFRK methods. Equation (41) can be rewritten as a conformal Hamiltonian system (31) with $z = [q, p]^T$, $p = \dot{q}$, and

$$H(q, p) = \tfrac{1}{2}(\kappa^2 q^2 + p^2 + \gamma qp).$$

To illustrate higher-order convergence, we apply stage 1, 2, and 3 GL-IFRK methods to (41) with γ constant. Figure 2 shows the ratio of local absolute error in solution and the step size as a function of the step size, which agrees with the theoretical local order of the methods.

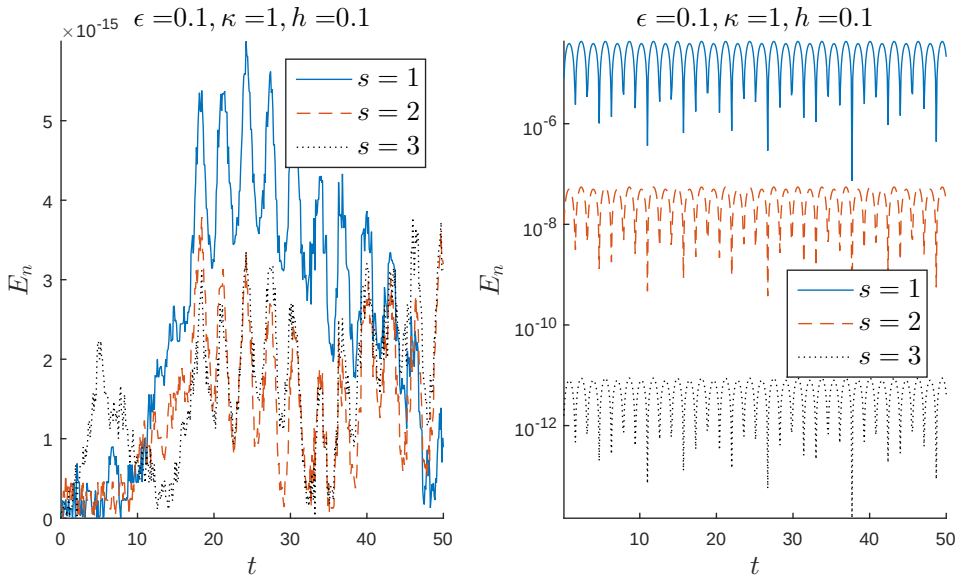

FIG. 3. *The error E_n (42) for the GL-IFRK methods (left) and the standard Gauss–Legendre methods (right) applied to* (41) *with* $\gamma(t) = \frac{1}{2}\varepsilon\cos(2t)$.

5.1.2. Time-dependent damping. Setting $\gamma(t) = \frac{1}{2}\varepsilon\cos(2t)$ with $\varepsilon \in \mathbb{R}$ in (41) yields a special case of Hill's equation, which is used to model rain-wind induced vibrations in an oscillator. Depending on parameter values, the solutions ($q : \mathbb{R} \to \mathbb{R}$) in this case may be periodic, bounded, or unbounded [11], providing richer solution behavior than the standard damped harmonic oscillator given in section 5.1.1.

An IFRK method for solving (41) is given by (5). Since $\varphi_0 = e^{-x_n(h)}$, we know that such methods satisfy the hypotheses of Corollary 4.6. Consequently, a numerical method with flow map $\Psi_h(z_n)$, which solves the system (31), is conformal symplectic if

$$E_n := \|(\Psi_h'(z_n))^T \mathbf{J}^{-1} \Psi_h'(z_n) - e^{-2\int_0^{t_{n+1}} \gamma(s)ds} \mathbf{J}^{-1}\| \tag{42}$$

vanishes. Since $z_{n+1} = \Psi_h(z_n)$ implies $dz_{n+1} = \Psi_h'(z_n)dz_n$, the Jacobian $\Psi_h'(z_n)$ can be computed by numerically solving the system for dz_{n+1}. For instance, the first two equations of the system (34) can be numerically solved for dQ, dP using exact methods or fixed point iterations and the resulting solutions can be substituted in the last two equations of the system to find dq_{n+1}, dp_{n+1}. In Figure 3, we plot the error E_n for both the GL-IFRK methods and the standard Gauss–Legendre methods of stages 1, 2, and 3, illustrating preservation of the property (39) by the GL-IFRK methods, but not for the standard methods.

5.2. Pendulum. Consider the pendulum problem

$$\ddot{q} + 2\gamma\dot{q} + \sin(q) = 0, \tag{43}$$

which is a conformal symplectic ODE. Using a real constant $\gamma > 1$, the pendulum is strongly damped. It can be shown that the differential equation satisfies

$$\frac{d}{dt}(\tfrac{1}{2}p^2 - \cos(q)) = -2\gamma p^2,$$

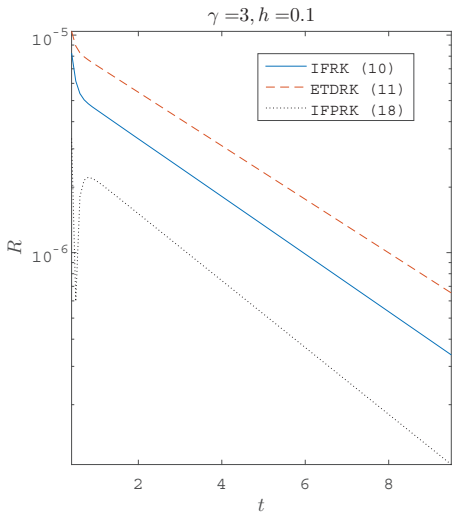

FIG. 4. *The residual* (44) *for three numerical solutions of* (43). *The methods used are IFRK* (10), *ETDRK* (11), *and IFPRK* (18).

which could be called the energy balance. Though this is not what we have called a conformal invariant for the system, it does provide a way to measure the accuracy of a method.

To this model problem, we apply the IFRK method (10), the IFPRK method (18), and the ETDRK method (11). All three methods are second order and conformal symplectic. The expression $(e^{\gamma h/2} - e^{-\gamma h/2})$ in (11) is evaluated by computing $2\sinh(\gamma h/2)$ instead. Denoting the eighth-order central finite difference operator by D_t, we plot the residual

$$R(t_n) = |D_t(\tfrac{1}{2}p_n^2 - \cos(q_n)) + 2\gamma p_n^2| \tag{44}$$

for each of the three methods in Figure 4. All the methods show rapid decay, but the PERK method produces smaller residuals, and the fact that it is explicit gives it a strong advantage.

It is important to note here that these differences between integrating factor and exponential time differencing methods are a result of choosing a relatively large value of γ. Other comparisons of interest with small damping coefficients do not often reveal such obvious differences between the methods. As a result, the integrating factor methods may often be preferable, because they are generally easier to construct and analyze.

5.3. Rigid body with periodic perturbation. Here, we present an example illustrating conformal quadratic invariant preservation by the ERK methods. Consider the following system of equations:

$$\begin{bmatrix} \dot{z_1} \\ \dot{z_2} \\ \dot{z_3} \end{bmatrix} = \begin{bmatrix} 0 & z_3/I_3 & -z_2/I_2 \\ -z_3/I_3 & 0 & z_1/I_1 \\ z_2/I_2 & -z_1/I_1 & 0 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} - \frac{\varepsilon}{2}\cos(2t) \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix}, \tag{45}$$

where I_1, I_2, I_3 are nonzero real constants and the term involving cosine function is a time-dependent damping term. When $\varepsilon = 0$, this system defines the motion of a

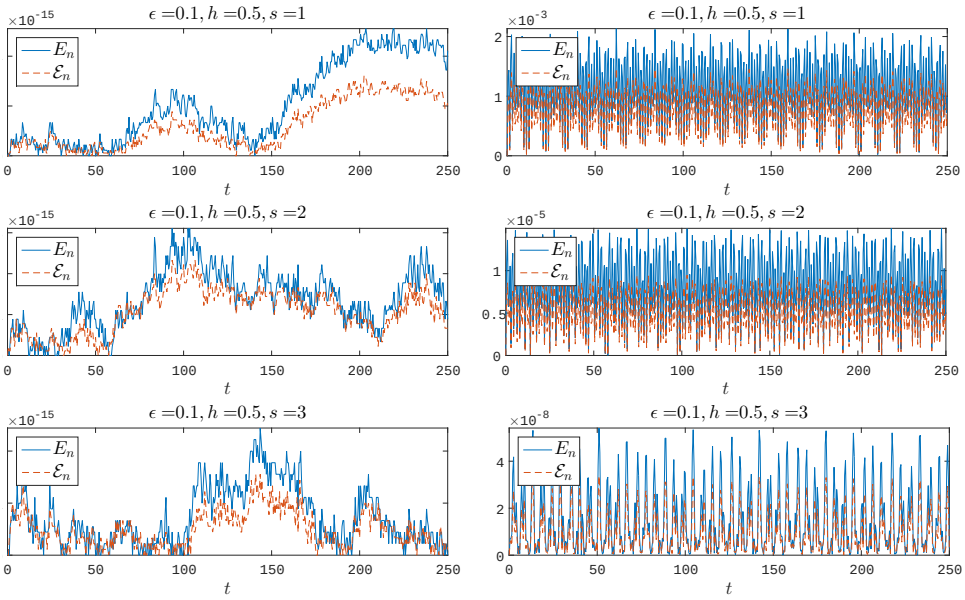

FIG. 5. *Casimir and energy errors* (46) *for simulations of the system* (45). *Left: GL-IFRK methods; Right: standard Gauss–Legendre methods.*

free rigid body with center of mass at the origin, the solution vector $z = (z_1, z_2, z_3)^T$ represents the angular momentum, and I_1, I_2, I_3 are principal moments of inertia. It is straightforward to show that solutions of the system satisfy two conformal quadratic invariants, one for the Casimir

$$\frac{dC}{dt} = -\varepsilon \cos(2t) C \qquad \text{with} \qquad C(z) = z_1^2 + z_2^2 + z_3^2$$

and one for the energy

$$\frac{dH}{dt} = -\varepsilon \cos(2t) H \qquad \text{with} \qquad H(z) = \frac{1}{2}\left(\frac{z_1^2}{I_1} + \frac{z_2^2}{I_2} + \frac{z_3^2}{I_3}\right).$$

Figure 5 shows plots of both

$$E_n = |C(z_n) - C(z_0) e^{-\frac{\varepsilon}{2}\sin(2t_n)}| \qquad \text{and} \qquad \mathcal{E}_n = |H(z_n) - H(z_0) e^{-\frac{\varepsilon}{2}\sin(2t_n)}|, \tag{46}$$

which are the residuals in Casimir and energy, respectively, and z_n is the numerical solution. The residuals from the standard Gauss–Legendre methods are proportional to the order of the method, but the figure verifies that the conformal quadratic invariants are preserved by the GL-IFRK methods.

6. Conclusions. This article presents and develops a class of exponential Runge–Kutta and partitioned exponential Runge–Kutta methods. The methods are useful for differential equations with solutions that satisfy properties of the form $\mathcal{I}(t) = e^{-x_0(t)}\mathcal{I}(0)$, where $\mathcal{I}$ is linear, quadratic, or a symplectic two-form. Because the methods produce solutions that satisfy $\mathcal{I}(t_{n+1}) = e^{-x_0(h)}\mathcal{I}(t_n)$ (under certain restrictions

on the coefficient functions), they preserve the properties in a way that is stronger than other methods that simply guarantee $\mathcal{I}(t_{n+1}) < \mathcal{I}(t_n)$ when $x_0(h) > 0$.

The nonconservative perturbations considered throughout the article have a special structure, and there are many important applications (listed in sections 3 and 5) that have this structure. On the other hand, the techniques presented here may not be fruitful for solving equations that do not have this special structure, though generalizations or extensions to other types of equations may be a topic for future research. The focus is on integrating factor methods and exponential time differencing methods, but the theorems on structure-preservation may also apply to other types of exponential integrators. The strengths of the methods are illustrated for various integrators applied to several model problems through numerical experiments.

The methods developed here are interesting for conservative systems that are perturbed with linear, possibly time-dependent, nonconservative terms, and many aspects of the methods are well-understood, thanks to a wealth of prior research on exponential integrators. Nevertheless, there are several avenues for future research on this topic, including order conditions for PERK methods, backward error analysis, extension and application to partial differential equations, and development of methods that preserve other important properties of mechanical systems that are perturbed by nonconservative terms.

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