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Abstract

Recently, the symplectic exponentially-fitted methods for Hamiltonian systems with periodic or oscillatory solutions have been attracting a lot of interest. As an alternative to them, in this paper, we propose a class of energy-preserving exponentially-fitted methods. For this aim, we show sufficient conditions for energy-preservation in terms of the coefficients of continuous stage Runge–Kutta methods, and extend the theory of exponentially-fitted Runge–Kutta methods in the context of continuous stage Runge–Kutta methods. Then by combining these two theories, we derive second and fourth order energy-preserving exponentially-fitted schemes.

Keywords
Continuous stage Runge–Kutta method Energy-preservation Exponential fitting Hamiltonian systems

1 Introduction

In this paper we consider numerical integration of Hamiltonian systems of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}y = J^{-1}\nabla H(y), \quad J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, \tag{1}$$

where $y \in \mathbb{R}^{2d}$, J is a skew-symmetric constant matrix with the identity matrix $I \in \mathbb{R}^{d\times d}$, and the Hamiltonian, which is also referred to as the energy, $H : \mathbb{R}^{2d} \to \mathbb{R}$ is assumed to be sufficiently differentiable. According to the result by Poincaré, the exact flow of Hamiltonian systems is for every t symplectic. Another important property of the flow is that it preserves energy, i.e., the Hamiltonian. In the spirit of geometric numerical integration, the ideal integrator would be that inherits such geometric properties as much as possible. But since a numerical integrator cannot inherit both symplecticity and energy-preservation [14, 57], methods satisfying each of these properties have been studied in the last decades. We call such methods symplectic or energy-preserving methods, respectively. It is widely accepted that such methods produce qualitatively nice numerical solutions over a long time (see [32, 36] for symplectic methods, and [32, 33] for energy-preserving methods, for example).

In a slightly different context, exponentially-fitted (EF) methods for ordinary differential equations with periodic or oscillatory solutions have been considered for deriving efficient algorithms making maximal use of available information on the solutions. Briefly speaking, EF methods are the methods that exactly integrate all functions of a given linear space that is chosen depending on the nature of the solutions of the original problem. For example, a numerical method which can exactly integrate all functions in a linear space $\{\cos(\omega t), \sin(\omega t)\}$ would be able to track $T = 2\pi/\omega$ periodic solutions more accurately than the standard methods even if $\omega \gg 1$. Such periodic or oscillatory solutions often arise in general Hamiltonian systems in different fields of applied sciences such as celestial mechanics, astrophysics, chemistry, electronics, molecular dynamics, and so on [1]. Therefore, for such Hamiltonian systems, it would be appropriate to consider symplectic or energy-preserving exponentially-fitted methods.

EF methods can be divided into two classes. The first class is based on linear multistep methods, and mainly focuses on second order differential equations. Methods in this class are also referred to as trigonometric methods. The second class is based on one-step methods, and aims at first order equations. Although the first class can be reformulated as one-step methods in principle, we basically distinguish these two classes because the constructions are completely different. The researches on the first class have a long history over fifty years, where a first good theoretical foundation was given by Gautschi [25] and Lyche [37]. Then in the last decades, trigonometric methods have been developed mainly in the context of highly oscillatory differential equations (see, for example, [16, 24, 27, 31, 32, 34, 48] and references therein). It is worth mentioning that some of the methods are symplectic [18, 24]. Compared to the above, the study of EF one-step methods is relatively new. In 1998, Paternoster [40] and Simos [45] constructed independently implicit and explicit EF one-step methods, respectively, based on the theory of Runge–Kutta (RK) methods. After that, the theory of so called exponentially-fitted RK (EFRK) methods has been developed by several authors [20, 21, 22, 38, 39, 40, 51, 52, 53, 55]. Recently, the theory of symplectic EFRK methods has been attracting much attention [7, 8, 9, 10, 11, 23, 49, 50, 54].

If we turn our attention to energy-preserving integrators, only a few papers ([56], for example) have been written in this context, and it seems much is left to be investigated. Taking these facts into account, in this paper we consider a construction of energy-preserving EF one-step methods. Below we clarify the difficulty of this challenge. The symplectic EF (one-step) methods have been constructed by the combination of the following theories:

- characterization of symplecticity in terms of the RK coefficients, and
- standard theory of EFRK methods.

From this, one might expect that energy-preserving EF methods can be constructed similarly by the combination of

- characterization of energy-preservation in terms of the RK coefficients, and
- standard theory of EFRK methods.

But such a combination is impossible because energy-preserving methods are not RK methods in general [13], and the first point above does not make sense at all unfortunately. The key to overcome this difficulty is to notice a recently discovered fact that certain classes of energy-preserving methods can be expressed as so called continuous stage RK (cRK) methods (Hairer [30] and Tang–Sun [47]). This can help constructing energy-preserving EF methods, and actually below we show that we can newly develop two theories:

- characterization of energy-preservation in terms of the cRK coefficients, and
- standard theory of EFcRK methods.

Here we stress that in the preceding studies, only the specific energy-preserving schemes were given, and the above first point has remained open so far. We also emphasize that as for the second point the extension is not straightforward, because we are forced to consider the different nodes from the EFRK methods on which the numerical solution is fitted to the given functions. Then we derive second and fourth order energy-preserving exponentially-fitted cRK (EPEFcRK) schemes making use of the two theories. We do not further get into higher order schemes, because the difficulty there seems to be not essential, but just technical.

This paper is organized as follows. In Section 2, we briefly review basic concepts of EFRK methods and summarize the construction of symplectic EFRK methods. In Section 3, we show sufficient conditions of energy-preservation in terms of the coefficients of cRK methods. Then we develop a theory of EF methods based on cRK methods (EFcRK methods), and derive energy-preserving EFcRK schemes. In Section 4, we show two numerical examples. Finally in Section 5 we conclude this paper with some discussion on the extension of the proposed method to Poisson systems and some comments on our future works.

In this paper we use several abbreviations. The following table shows their list.

RK	Runge–Kutta
EF	exponential-fitting, exponentially-fitted
FF	functional-fitting, functionally-fitted
SEFRK	symplectic exponentially-fitted Runge–Kutta
cRK	continuous stage Runge–Kutta
EPcRK	energy-preserving continuous stage Runge–Kutta
EFcRK	exponentially-fitted continuous stage Runge–Kutta
EPEFcRK	energy-preserving exponentially-fitted continuous stage Runge–Kutta

2 A brief review of exponentially fitted RK methods and symplectic exponentially-fitted RK methods

In this section, we briefly review basic concepts of the EFRK methods and summarize the construction of SEFRK methods.

2.1 Characterizations of symplecticity and symmetry of RK methods

As is well known, the s-stage Gauss method is a symplectic and symmetric RK method with the accuracy of order $2s$. Most of the existing implicit EFRK methods with even order can be seen as extensions of the Gauss method. In order to review SEFRK methods in this section, we first summarize the characterizations of symplecticity and symmetry in terms of the RK methods, which play a crucial role in constructing SEFRK methods. For more details, see [32, 36, 44] for example.

We consider an s-stage modified RK (mRK) method defined by

$$Y_i = \gamma_i y_0 + h \sum_{j=1}^{s} a_{ij} f(Y_j), \quad i = 1, \dots, s, \tag{2}$$

$$y_1 = \phi_h(y_0) = y_0 + h\sum_{i=1}^{s} b_i f(Y_i), \tag{3}$$

where $y_1 \approx y(t_0+h)$, $Y_i \approx y(t_0+c_ih)$ $(i=1,\dots,s)$ and the real parameters c_i and b_i $(i=1,\dots,s)$ denote the nodes and the weights of the method. In the standard RK methods, all $\gamma_i = 1$, but several authors introduced γ_i's in the context of exponential fitting [20, 51, 52] (see Section 2.3). We often refer to (2) and (3) as internal and final stages, respectively. The mRK method (2) and (3) is often represented by means of Butcher's tableau

$$\begin{array}{c|c|c} \boldsymbol{c} & \boldsymbol{\gamma} & \boldsymbol{A} \\ \hline & & \boldsymbol{b}^\top \end{array} = \begin{array}{c|c|ccc} c_1 & \gamma_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & \gamma_s & a_{s1} & \cdots & a_{ss} \\ \hline & & b_1 & \cdots & b_s \end{array}$$

or equivalently the quartet $(\boldsymbol{c}, \boldsymbol{\gamma}, \boldsymbol{A}, \boldsymbol{b})$.

The exact flow, denoted by $\psi_t(y_0)$, of the Hamiltonian system (1) is symplectic for every t. This means that the Jacobian matrix of $\psi_t(y_0)$ satisfies

$$\psi_t'(y_0)^\top J \psi_t'(y_0) = J.$$

A numerical method defined by the flow map ϕ_h is called symplectic if for all Hamiltonian systems (1) it satisfies the condition

$$\phi_h'(y_0)^\top J \phi_h'(y_0) = J.$$

In general, it is advantageous to adopt symplectic methods in terms of the long time behaviour. This can be verified by backward error analyses. The conditions for a RK method being symplectic were obtained independently by Lasagni, Sanz-Serna and Suris (see [32, 35, 43, 44, 46] and references therein), and as an extension of them, those of a mRK method were obtained by Van de Vyver [49, 50].

Theorem 2.1 ([49, 50])**.** A mRK method solving Hamiltonian systems is symplectic if the following conditions are satisfied

$$b_j\frac{a_{ji}}{\gamma_j} + b_i\frac{a_{ij}}{\gamma_i} - b_ib_j = 0, \quad 1 \le i,j \le s.$$

Symmetry is also an important concept because the accuracy order of a symmetric method is even. The adjoint method ϕ_h^* of a numerical method ϕ_h is the inverse map of the original method with the reversed time step $-h$, i.e., $\phi_h^* := \phi_{-h}^{-1}$. In other words, $y_1 = \phi_h^*(y_0)$ is implicitly defined by $\phi_{-h}(y_1) = y_0$. A method satisfying $\phi_h^* = \phi_h$ is called symmetric. In [7], for mRK methods whose coefficients are even functions of h, the symmetry conditions are given by

$$\boldsymbol{c} + S\boldsymbol{c} = e, \quad \boldsymbol{b} = S\boldsymbol{b}, \quad \boldsymbol{\gamma} = S\boldsymbol{\gamma}, \quad S\boldsymbol{A} + \boldsymbol{A}S = \boldsymbol{\gamma}\boldsymbol{b}^\top, \tag{4}$$

where

$$\boldsymbol{e} = (1,\dots,1)^\top \in \mathbb{R}^s \quad \text{and } S = (s_{ij}) \in \mathbb{R}^{s\times s} \quad \text{with } s_{ij} = \begin{cases} 1, & \text{if } i+j = s+1, \\ 0, & \text{otherwise.} \end{cases}$$

2.2 Exponentially-fitted RK methods

In this subsection, we briefly review basic concepts of the exponentially-fitted RK (EFRK) methods. Recently, a collocation approach for constructing RK methods which exactly integrates a set of linearly independent functions (not necessarily polynomials) has been developed. The main idea consists in choosing the available parameters of the method (2)–(3), i.e., $\boldsymbol{c}$, $\boldsymbol{\gamma}$, $\boldsymbol{A}$ and $\boldsymbol{b}$, such that the resulting scheme is exact for a set of linearly independent scalar functions in $[t_0, t_0 + h]$

$$\mathcal{F} = \{u_1(t), u_2(t), \ldots, u_r(t)\}, \quad r \leq s.$$

We often refer to this set as the reference set. Originally, the set $\mathcal{F} = \{1, t, t^2, \ldots, t^s\}$ was considered, where the parameters of the resulting scheme is independent of h. If $\mathcal{F}$ contains exponential or trigonometric functions, these methods are called EFRK methods. In more general cases in which $\mathcal{F}$ contains general functions, these methods are called functionally-fitted RK (FFRK) methods [38, 39]. In general, the coefficients $(\boldsymbol{c}, \boldsymbol{\gamma}, \boldsymbol{A}, \boldsymbol{b})$ of an EFRK or FFRK method may depend on not only the fitting functions $u_1, \ldots, u_r$, but also the step size h. The coefficients of a FFRK method (2)–(3) are determined by the linear systems

$$u_k(t_0\boldsymbol{e} + h\boldsymbol{c}) - \boldsymbol{\gamma} u_k(t_0) = h\boldsymbol{A} u_k'(t_0\boldsymbol{e} + h\boldsymbol{c}), \quad k = 1, \ldots, r, \tag{5}$$

$$u_k(t_0 + h) - u_k(t_0) = h\boldsymbol{b}^\top u_k'(t_0\boldsymbol{e} + h\boldsymbol{c}), \qquad k = 1, \ldots, r, \tag{6}$$

where $\boldsymbol{e} = (1, \ldots, 1)^\top \in \mathbb{R}^s$ and we use the notation $g(\boldsymbol{v}) = (g(v_1), \ldots, g(v_s))^\top$ for $\boldsymbol{v} = (v_1, \ldots, v_s) \in \mathbb{R}^s$ and a scalar function g.

In general cases, the coefficients may depend on t_0, h and $\mathcal{F}$, but under some usual requirements on $\mathcal{F}$, they are independent of t_0. In this paper we will consider only such usual cases.

Let us consider the solvability of the systems (5) and (6). When $r = s$, the coefficients $\boldsymbol{b}$ and $\boldsymbol{A}$ are uniquely determined for all $h > 0$ and $t \in [t_0, T]$, if the matrix

$$M(t, h) = \begin{pmatrix} u_1'(t + c_1 h) & \cdots & u_1'(t + c_s h) \\ \vdots & \ddots & \vdots \\ u_s'(t + c_1 h) & \cdots & u_s'(t + c_s h) \end{pmatrix}$$

is non-singular [38]. Below we sum up the key idea of the proof of this statement. If the functions $u_k(t)$ $(k = 1, \ldots, s)$ are sufficiently smooth, from the Taylor expansion we have

$$M(t, h) = W^\top(t) \begin{pmatrix} 1 & 1 & \cdots & 1 \\ c_1 h & c_2 h & \cdots & c_s h \\ \vdots & \vdots & \ddots & \vdots \\ \frac{(c_1 h)^{s-1}}{(s-1)!} & \frac{(c_2 h)^{s-1}}{(s-1)!} & \cdots & \frac{(c_s h)^{s-1}}{(s-1)!} \end{pmatrix} + \mathcal{O}(h^s), \tag{7}$$

where $W(t)$ is the Wronskian matrix defined by

$$W(t) := \begin{pmatrix} u_1'(t) & \cdots & u_s'(t) \\ \vdots & \ddots & \vdots \\ u_1^{(s)}(t) & \cdots & u_s^{(s)}(t) \end{pmatrix}, \quad \left(u^{(i)} := \frac{\mathrm{d}^i}{\mathrm{d}t^i} u(t) \right).$$

Therefore, due to the continuity of determinant, if the nodes are different ($c_i \neq c_j$, $i \neq j$) and $W(t)$ is non-singular, the coefficients $\boldsymbol{b}$ and $\boldsymbol{A}$ are uniquely determined.

In the context of EFRK methods, we usually consider

$$\mathcal{F}_1 = \{\exp(\lambda t), \exp(-\lambda t)\} \tag{8}$$

or $\mathcal{F}_2 = \{\cos(\omega t), \sin(\omega t)\}$. Note that $\mathcal{F}_2$ is obtained from $\mathcal{F}_1$ with $\lambda = i\omega$. When we consider the reference set $\mathcal{F}_1$, the linear systems (5)–(6) reduce to

$$\begin{aligned} \boldsymbol{A}\cosh(\boldsymbol{c}z) &= \frac{\sinh(\boldsymbol{c}z)}{z}, \quad \boldsymbol{A}\sinh(\boldsymbol{c}z) = \frac{\cosh(\boldsymbol{c}z) - \boldsymbol{\gamma}}{z}, \\ \boldsymbol{b}^\top\cosh(\boldsymbol{c}z) &= \frac{\sinh(z)}{z}, \quad \boldsymbol{b}^\top\sinh(\boldsymbol{c}z) = \frac{\cosh(z) - 1}{z}, \end{aligned}$$

where $z = \lambda h$. For $s = 2$, by the above statement, the coefficients $\boldsymbol{b}$ and $\boldsymbol{A}$ are uniquely determined in terms of the nodes $\boldsymbol{c}$ and parameters $\boldsymbol{\gamma}$. By simply choosing the Gaussian nodes $(c_1, c_2) = (\frac{1}{2} - \frac{\sqrt{3}}{6}, \frac{1}{2} + \frac{\sqrt{3}}{6})$ and $\gamma_1 = \gamma_2 = 1$, we can obtain the fourth order EFRK method which reduces to the two-stage Gauss method when $\lambda = 0$ [55]. Unfortunately, however, this method is not symplectic as shown in [11], which indicates that the derivation of symplectic EFRK methods needs some more tricks.

2.3 Symplectic exponentially-fitted RK methods

Recently, some symplectic (and symmetric) EFRK (SEFRK) methods has been proposed by several authors. In Table 1, some existing methods are shown.

Table 1: SEF methods.

2nd order	Van de Vyver [49]
4th order	Vyver [50], Calvo et al. [8]
6th order	Calvo et al. [7, 9]
8th order	Calvo et al. [11], Vanden Berghe–Van Daele [54]
$2s$ order	Calvo et al. [10]

We illustrate here the key for the construction of SEFRK methods, following [8]. By taking the derivation of fourth order SEFRK scheme as our example, let us start with a two stage mRK formulation

$$\begin{array}{c|c|cc} c_1 & \gamma_1 & a_{11} & a_{12} \\ c_2 & \gamma_2 & a_{21} & a_{22} \\ \hline & & b_1 & b_2 \end{array}.$$

The coefficients should be related by

$$\begin{array}{c|c|cc} c_1 & \gamma_1 & a_{11} & a_{12} \\ c_2 & \gamma_2 & a_{21} & a_{22} \\ \hline & & b_1 & b_2 \end{array} = \begin{array}{c|c|cc} \frac{1}{2} - \theta & \gamma & \frac{\gamma b}{2} & a \\ \frac{1}{2} + \theta & \gamma & \gamma b - a & \frac{\gamma b}{2} \\ \hline & & b & b \end{array} \tag{9}$$

for the method being symplectic and symmetric. Here Theorem 2.1 and (4) were used.

When we consider the reference set of functions $\mathcal{F}_1$ (8), the linear systems (5)–(6) reduce to

$$\boldsymbol{A}\cosh(\boldsymbol{c}z) = \frac{\sinh(\boldsymbol{c}z)}{z}, \quad \boldsymbol{A}\sinh(\boldsymbol{c}z) = \frac{\cosh(\boldsymbol{c}z) - \boldsymbol{\gamma}}{z}, \tag{10}$$

$$\boldsymbol{b}^\top\cosh(\boldsymbol{c}z) = \frac{\sinh(z)}{z}, \quad \boldsymbol{b}^\top\sinh(\boldsymbol{c}z) = \frac{\cosh(z) - 1}{z}, \tag{11}$$

where $z = \lambda h$. Firstly, from $b_1 = b_2 = b$, $c_{1,2} = \frac{1}{2} \mp \theta$, and (11), we can easily obtain

$$b_1 = b_2 = b = \frac{\sinh(\frac{z}{2})}{z\cosh(\theta z)}.$$

Next, from $\gamma_1 = \gamma_2 = \gamma$ and (10), the coefficients $\boldsymbol{A}$ are given by

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \frac{1}{z\sinh(2\theta z)} \begin{pmatrix} \gamma\cosh((\frac{1}{2}+\theta)z) - \cosh(2\theta z) & 1 - \gamma\cosh((\frac{1}{2}-\theta)z) \\ -1 + \gamma\cosh((\frac{1}{2}+\theta)z) & -\gamma\cosh((\frac{1}{2}-\theta)z) + \cosh(2\theta z) \end{pmatrix}.$$

The parameter γ can be also determined as

$$\gamma_1 = \gamma_2 = \gamma = \frac{2\cosh(2\theta z)}{\cosh((\frac{1}{2}+\theta)z) + \cosh((\frac{1}{2}-\theta)z)}$$

in order to satisfy the relation (9). Finally we select the parameter θ using the order conditions. The resulting scheme is of order four if $\theta = \sqrt{3}/6$. This fourth order SEFRK scheme coincides with that obtained in [50].

Remark 2.2. As pointed out in almost all papers dealing with EF methods, the coefficients are subject to heavy cancellation when evaluated for small values of $|z|$. In that case the following series expansions should be used:

$$\begin{aligned}
a_{11} &= a_{22} = \frac{1}{4} - \frac{7}{8640}z^4 + \frac{31}{272160}z^6 - \frac{167}{13063680}z^8 + \cdots, \\
a_{12} &= \frac{1}{4} - \frac{\sqrt{3}}{6} + \frac{\sqrt{3}}{216}z^2 - \left(\frac{7}{8640} + \frac{\sqrt{3}}{6480}\right)z^4 + \left(\frac{31}{272160} + \frac{17\sqrt{3}}{3265920}\right)z^6 \\
&\quad - \left(\frac{167}{13063680} + \frac{31\sqrt{3}}{176359680}\right)z^8 + \cdots, \\
a_{21} &= \frac{1}{4} + \frac{\sqrt{3}}{6} - \frac{\sqrt{3}}{216}z^2 + \left(-\frac{7}{8640} + \frac{\sqrt{3}}{6480}\right)z^4 + \left(\frac{31}{272160} - \frac{17\sqrt{3}}{3265920}\right)z^6 \\
&\quad + \left(-\frac{167}{13063680} + \frac{31\sqrt{3}}{176359680}\right)z^8 + \cdots, \\
\gamma &= 1 - \frac{1}{288}z^4 + \frac{1}{2160}z^6 - \frac{881}{17418240}z^8 + \cdots \\
b &= \frac{1}{2} + \frac{1}{8640}z^4 - \frac{1}{272160}z^6 + \frac{13}{104509440}z^8 + \cdots.
\end{aligned}$$

It is clear that in the limit $z \to 0$ the well known classical fourth-order Gauss method is recovered.

3 Continuous stage RK methods and energy-preserving continuous stage RK methods

In this section, we develop two theories:

- characterization of energy-preservation (and symmetry) in terms of cRK coefficients (in Section 3.1),
- standard theory of EFcRK methods (in Section 3.2),

and derive second and fourth order energy-preserving exponentially-fitted cRK (EPEFcRK) schemes (in Section 3.3) making use of the two theories.

3.1 Continuous stage RK methods and their characterizations of energy-preservation and symmetry

For Hamiltonian systems (1), the Hamiltonian $H(y(t))$ is constant along the solution, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}H(y(t)) = 0.$$

A numerical method defined by the flow map ϕ_h is called energy-preserving if for all Hamiltonian systems (1) it satisfies the condition

$$H(\phi_h(y_0)) = H(y_0).$$

The simplest way to derive energy-preserving methods is to apply the projection method ([2, 3, 4, 17, 19, 28, 29], and their references therein). But it is now recognized that the discrete gradient method [26, 42] is the most standard framework and in most cases produces better numerical solutions. As a special case for obtaining a discrete gradient, Quispel–McLaren proposed the average vector field (AVF) method [41] which is widely used these days. The AVF method reads

$$y_1 = y_0 + hJ^{-1}\int_0^1 \nabla H((1-\tau)y_0 + \tau y_1)\mathrm{d}\tau. \tag{12}$$

From the chain rule and the skew-symmetry of J, we have

$$\begin{aligned}
&H(y_1) - H(y_0)\\
&= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\tau}H((1-\tau)y_0 + \tau y_1)\mathrm{d}\tau\\
&= h\left(\frac{y_1 - y_0}{h}\right)^{\top}\int_0^1 \nabla H((1-\tau)y_0 + \tau y_1)\mathrm{d}\tau\\
&= h\left(\int_0^1 \nabla H((1-\tau)y_0 + \tau y_1)\mathrm{d}\tau\right)^{\top} J^{-\top}\left(\int_0^1 \nabla H((1-\tau)y_0 + \tau y_1)\mathrm{d}\tau\right) = 0.
\end{aligned}$$

Therefore, the AVF method is energy-preserving and clearly of order two. Obviously, this method is not a RK method. Moreover, as shown by Celledoni et al. [12, Proposition 4], no RK method is energy-preserving in general.

The AVF method (12) and its generalization to high-order can be expressed as cRK methods [32, 47]. We consider an s-degree cRK method defined by

$$Y_\tau = y_0 + h\int_0^1 A_{\tau,\sigma} f(Y_\sigma)\mathrm{d}\sigma, \tag{13}$$

$$y_1 = y_0 + h\int_0^1 B_\sigma f(Y_\sigma)\mathrm{d}\sigma, \tag{14}$$

where Y_τ is a polynomial of degree s with respect to τ satisfying $Y_0 = y_0$, and $A_{\tau,\sigma}$ and B_σ are polynomial with respect to the variables in the subscripts. For example, when $s = 1$, $A_{\tau,\sigma} = \tau$, and $B_\sigma = 1$, the cRK method (13)–(14) reduces to the AVF method (12). Below, for simplicity, we restrict our consideration to $A_{\tau,\sigma}$ of degree s for τ, and $s-1$ for σ.

Recall that in a mRK method the internal (2) and final (3) stages can be treated independently in principle. In other words, the coefficients $\boldsymbol{A}$ and $\boldsymbol{b}$ can be chosen independently. Of course, the internal stages (13) and final stage (14) correspond to those of the mRK method. However, in a cRK method, there is a restrictive relation between the internal and final stages for the consistency of the method, because y_1 should coincide with Y_1. Therefore, B_σ should be expressed as $B_\sigma = A_{1,\sigma}$.

Let us introduce the following tableau

$$\begin{array}{ccc} a_{11} & \cdots & a_{1q} \\ \vdots & \ddots & \vdots \\ a_{p1} & \cdots & a_{pq} \\ \hline b_1 & \cdots & b_q \end{array}$$

where a_{ij} and b_j denote the coefficients in terms of $\tau^i\sigma^{j-1}$ and σ^{j-1}, respectively. The condition $B_\sigma = A_{1,\sigma}$ is equivalent to

$$b_j = \sum_{i=1}^{p} a_{ij}.$$

In this paper, we consider only the case $p = q = s$.

Although cRK methods were introduced in the context of energy-preserving methods [13, 30, 47], the characterization of energy-preservation has not yet known. In the following theorem, we show sufficient conditions of energy-preservation in terms of the coefficient $A_{\tau,\sigma}$.

Theorem 3.1. A cRK method solving Hamiltonian systems is energy-preserving if $\frac{\mathrm{d}}{\mathrm{d}\tau}A_{\tau,\sigma}$ is symmetric, i.e.,

$$A'_{\tau,\sigma} = A'_{\sigma,\tau} \quad \text{where } A'_{\tau,\sigma} := \frac{\mathrm{d}}{\mathrm{d}\tau}A_{\tau,\sigma}. \tag{15}$$

Proof. We can express $(\mathrm{d}/\mathrm{d}\tau)A_{\tau,\sigma}$ as

$$\frac{\mathrm{d}}{\mathrm{d}\tau}A_{\tau,\sigma} = \sum_{l=0}^{s-1} a'(l,l)\tau^l\sigma^l + \sum_{m<n}\big(a'(m,n)\tau^m\sigma^n + a'(n,m)\tau^n\sigma^m\big).$$

Note that the symmetry of $(\mathrm{d}/\mathrm{d}\tau)A_{\tau,\sigma}$ is equivalent to $a'(m,n) = a'(n,m)$. Thus we have

$$H(y_1) - H(y_0) = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\tau}H(Y_\tau)\mathrm{d}\tau = \int_0^1 \dot{Y}_\tau^{\top}\nabla H(Y_\tau)\mathrm{d}\tau$$

$$
\begin{aligned}
&= h\int_0^1 \left(\int_0^1 \frac{\mathrm{d}}{\mathrm{d}\tau} A_{\tau,\sigma} J^{-1}\nabla H(Y_\sigma)\mathrm{d}\sigma\right)^\top \nabla H(Y_\tau)\mathrm{d}\tau \\
&= h\sum_{l=0}^{s-1} a'(l,l)\left(\int_0^1 \sigma^l \nabla H(Y_\sigma)\mathrm{d}\sigma\right)^\top J^{-\top}\int_0^1 \tau^l \nabla H(Y_\tau)\mathrm{d}\tau \\
&\quad + h\sum_{m<n}\left\{a'(m,n)\left(\int_0^1 \sigma^n \nabla H(Y_\sigma)\mathrm{d}\sigma\right)^\top J^{-\top}\int_0^1 \tau^m \nabla H(Y_\tau)\mathrm{d}\tau\right. \\
&\qquad \left. + a'(n,m)\left(\int_0^1 \sigma^m \nabla H(Y_\sigma)\mathrm{d}\sigma\right)^\top J^{-\top}\int_0^1 \tau^n \nabla H(Y_\tau)\mathrm{d}\tau\right\} = 0.
\end{aligned}
$$

In the last equality, the first term vanishes due to the skew-symmetry of J. The second term vanishes because of

$$
\begin{aligned}
&\left(\int_0^1 \sigma^n \nabla H(Y_\sigma)\mathrm{d}\sigma\right)^\top J^{-\top}\int_0^1 \tau^m \nabla H(Y_\tau)\mathrm{d}\tau \\
&= -\left(\int_0^1 \sigma^m \nabla H(Y_\sigma)\mathrm{d}\sigma\right)^\top J^{-\top}\int_0^1 \tau^n \nabla H(Y_\tau)\mathrm{d}\tau
\end{aligned}
$$

and the symmetry $a'(m,n) = a'(n,m)$. □

As shown in [30], the symmetry condition of a cRK method whose coefficients are even functions of h can be written as

$$
A_{1-\tau,1-\sigma} + A_{\tau,\sigma} = B_\sigma. \tag{16}
$$

The known coefficients $A_{\tau,\sigma}$ of 2nd, 4th and 6th order EP schemes in [30] satisfy the conditions of the above theorem and (16).

- 2nd order EP scheme ($s = 1$): $A_{\tau,\sigma} = \tau$,
- 4th order EP scheme ($s = 2$): $A_{\tau,\sigma} = \tau((4-3\tau) - 6(1-\tau)\sigma)$,
- 6th order EP scheme ($s = 3$): $A_{\tau,\sigma} = \tau((9-18\tau+10\tau^2) - 12(3-8\tau+5\tau^2)\sigma + 30(1-3\tau+2\tau^2)\sigma^2)$.

They can be rewritten as follows.

$$
\begin{array}{c|c}
1 & 1 \\ \hline
 & 1
\end{array},\quad
\begin{array}{cc|c}
4 & -6 & \\
-3 & 6 & \\ \hline
1 & 0 &
\end{array},\quad
\begin{array}{ccc|c}
9 & -36 & 30 & \\
-18 & 96 & -90 & \\
10 & -60 & 60 & \\ \hline
1 & 0 & 0 &
\end{array}.
$$

3.2 Exponentially-fitted cRK methods

In this subsection, we develop a theory of standard EFcRK methods. But we consider a wider class of functionally-fitted cRK (FFcRK) methods which contain EFcRK methods as special cases. For s-stage FFRK methods, we can consider the fitting on $s+1$ nodes, i.e., $t = t_0 + c_1 h, \ldots, t_0 + c_s h, t_0 + h$, because the coefficients $\boldsymbol{A}$ and $\boldsymbol{b}$ can be chosen independently. However, for s-degree FFcRK methods, since $A_{\tau,\sigma}$ and B_σ are dependent, we can consider the fitting on only s nodes, and one of them should be $t = t_0 + h$. This fact is the biggest difference between FFRK methods and FFcRK methods.

The coefficients $A_{\tau,\sigma}$ and B_σ of a FFcRK method are determined by the linear systems

$$u_k(t_0\boldsymbol{e}+h\boldsymbol{c})-u_k(t_0)=h\int_0^1 A_{\boldsymbol{c},\sigma}\widetilde{u_k'}(t_0+\sigma h)\mathrm{d}\sigma,\quad k=1,\dots,r, \tag{17}$$

$$u_k(t_0\boldsymbol{e}+h)-u_k(t_0)=h\int_0^1 B_\sigma\widetilde{u_k'}(t_0+\sigma h)\mathrm{d}\sigma,\qquad k=1,\dots,r, \tag{18}$$

where $\boldsymbol{c}=(c_1,\dots c_{s-1})^\top\in\mathbb{R}^{s-1}$, $\boldsymbol{e}=(1,\dots,1)^\top\in\mathbb{R}^{s-1}$. Here we also introduced the following notation: for a scalar function g and a vector $\boldsymbol{v}=(v_1,\dots,v_{s-1})^\top\in\mathbb{R}^{s-1}$, $g(\boldsymbol{v})$ means the abbreviation $g(\boldsymbol{v})=(g(v_1),\dots,g(v_{s-1}))^\top$, and $\widetilde{g}(t_0+\sigma h)$ denotes a polynomial of degree s which is a linear combination of $g(t_0),g(t_0+c_1h),\dots,g(t_0+c_{s-1}h),g(t_0+h)$.

Proposition 3.2. *Assume that $u_1,\dots,u_r$ are sufficiently smooth. When $r=s$, the coefficients $A_{\tau,\sigma}$ are uniquely determined for all h and $t\in[t_0,T]$ if the Wronskian matrix*

$$W(t):=\begin{pmatrix}u_1'(t) & \cdots & u_s'(t)\\ \vdots & \ddots & \vdots\\ u_1^{(s)}(t) & \cdots & u_s^{(s)}(t)\end{pmatrix}$$

is non-singular and the nodes $0<c_1,\dots,c_{s-1}<1$ are different.

Proof. Since $A_{\boldsymbol{c},\sigma}$ and $\widetilde{u_k'}(t_0+\sigma h)$ are polynomials of degree $s-1$ and s in terms of σ, the right hand side of (17) can be integrated exactly by the s-points Gaussian quadrature rule:

$$h\int_0^1 A_{c_i,\sigma}\widetilde{u_k'}(t_0+\sigma h)\mathrm{d}\sigma=h\sum_{j=1}^s b_j'A_{c_i,c_j'}\widetilde{u_k'}(t_0+c_j'h)$$

where c_j' $(j=1,\dots,s)$ denote the Gaussian nodes and

$$b_i'=\int_0^1\prod_{j=1,j\neq i}^s\frac{\tau-c_j'}{c_i'-c_j'}\mathrm{d}\tau.$$

Therefore if the matrix

$$\begin{pmatrix}\widetilde{u_1'}(t+c_1'h) & \cdots & \widetilde{u_1'}(t+c_s'h))\\ \vdots & \ddots & \vdots\\ \widetilde{u_s'}(t+c_1'h) & \cdots & \widetilde{u_s'}(t+c_s'h)\end{pmatrix} \tag{19}$$

is non-singular, $A_{c_i,c_j'}$ are uniquely determined. Moreover if the nodes $0<c_1,\dots,c_{s-1}<1$ are different, the coefficients of $A_{\tau,\sigma}$ are also uniquely determined.

Obviously the non-singularity of the matrix (19) is equivalent to that of $M(t,h)$ in (7). Following the discussion there, we can conclude that if the Wronskian matrix is non-singular, the matrix (19) is also non-singular. This completes the proof. □

3.3 Derivation of energy-preserving exponentially-fitted cRK schemes

In this subsection, we derive second and fourth order EPEFcRK schemes. In what follows, we again consider $\mathcal{F}_1=\{\exp(\lambda t),\exp(-\lambda t)\}$.

3.3.1 Second order EPEFcRK scheme

Let us start with a one-degree cRK formulation: $A_{\tau,\sigma} = a_{11}\tau$. In this case, the EP and symmetry conditions are automatically satisfied. Therefore, the only thing we have to do is to determine the parameter a_{11} satisfying the EF conditions. When we consider the reference set $\mathcal{F}_1$ (8), the linear system (18) reduces to

$$\mathrm{e}^z = 1 + a_{11} z \frac{1+\mathrm{e}^z}{2}, \quad \mathrm{e}^{-z} = 1 - a_{11} z \frac{1+\mathrm{e}^{-z}}{2},$$

where $z = \lambda h$. We can easily obtain

$$a_{11} = \frac{2\sinh(\frac{z}{2})}{z\cosh(\frac{z}{2})},$$

and the resulting scheme reads

$$y_1 = y_0 + a_{11} h \int_0^1 f((1-\sigma)y_0 + \sigma y_1)\mathrm{d}\sigma.$$

When we implement the scheme, if the value $|z|$ is small, the following series expansion should be used:

$$a_{11} = 1 - \frac{1}{12}z^2 + \frac{1}{120}z^4 - \frac{17}{20160}z^6 + \frac{31}{362880}z^8 - \frac{691}{79833600}z^{10} + \frac{5461}{6227020800}z^{12} + \cdots.$$

It is clear that in the limit $z \to 0$ the well known AVF method (12) is recovered.

3.3.2 Fourth order EPEFcRK scheme

Let us start with a two-degree cRK formulation:

$$A_{\tau,\sigma} = a_{11}\tau + a_{12}\tau\sigma + a_{21}\tau^2 + a_{22}\tau^2\sigma.$$

Firstly, we consider the EP and symmetry conditions. The EP condition (15) is equivalent to

$$a_{12} = 2a_{21},$$

and the symmetry condition (16) is equivalent to

$$a_{22} + 2a_{21} = 0, \quad a_{22} + a_{12} = 0.$$

Therefore, it follows that a two-degree cRK method whose coefficients are related by

$$\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \\ \hline b_1 & b_2 \end{array} = \begin{array}{cc} a_{11} & 2a_{21} \\ a_{21} & -2a_{21} \\ \hline a_{11}+a_{21} & 0 \end{array} \tag{20}$$

is energy-preserving and symmetric.

Next we consider the EF conditions. We write Y_τ as a linear combination of y_0, Y_c and y_1, i.e.,

$$Y_\tau = y_0 \frac{(\tau-c)(\tau-1)}{c} + Y_c \frac{\tau(\tau-1)}{c(c-1)} + y_1 \frac{\tau(\tau-c)}{1-c}.$$

Then the method becomes

$$Y_c = y_0 + h\int_0^1 A_{c,\sigma} f(Y_\sigma)\mathrm{d}\sigma,$$
$$y_1 = y_0 + h\int_0^1 B_\sigma f(Y_\sigma)\mathrm{d}\sigma.$$

Note that although y_1 is independent of c in standard cRK methods, the parameter c plays an important role in EFcRK methods.

When we consider the reference set $\mathcal{F}_1$ (8), the linear systems (17) and (18) reduce to

$$\int_0^1 A_{c,\sigma}\widetilde{\cosh}(\sigma z)\mathrm{d}\sigma = \frac{\sinh(cz)}{z}, \quad \int_0^1 A_{c,\sigma}\widetilde{\sinh}(\sigma z)\mathrm{d}\sigma = \frac{\cosh(cz)-1}{z}, \tag{21}$$
$$\int_0^1 B_\sigma\widetilde{\cosh}(\sigma z)\mathrm{d}\sigma = \frac{\sinh(z)}{z}, \quad \int_0^1 B_\sigma\widetilde{\sinh}(\sigma z)\mathrm{d}\sigma = \frac{\cosh(z)-1}{z}, \tag{22}$$

where $z = \lambda h$, $\widetilde{\cosh}(\sigma z)$ denotes a polynomial of degree two which is a linear combination of $\cosh(0)$, $\cosh(cz)$ and $\cosh(z)$, and the similar notation is used for sinh. Since B_σ is independent of σ (see (20)), the second conditions (22) are equivalent to

$$B_\sigma\frac{(3c^2-4c+1)-\cosh(cz)+(3c^2-2c)\cosh(z)}{6c^2-6c} = \frac{\sinh(z)}{z},$$
$$B_\sigma\frac{-\sinh(cz)+(3c^2-2c)\sinh(z)}{6c^2-6c} = \frac{\cosh(z)-1}{z}.$$

We obtain $c = 1/2$ from the compatibility condition

$$\frac{(3c^2-4c+1)-\cosh(cz)+(3c^2-2c)\cosh(z)}{\sinh(z)} = \frac{-\sinh(cz)+(3c^2-2c)\sinh(z)}{\cosh(z)-1}$$
$$\Leftrightarrow \quad (2c-1)(1-\cosh(z)) + 2\sinh\left(\frac{z}{2}\right)\sinh\left(\frac{(2c-1)z}{2}\right) = 0,$$

and then have

$$B_\sigma = a_{11} + a_{21} = \frac{6(\cosh(z)-1)}{z\big(4\sinh(\frac{z}{2})+\sinh(z)\big)}. \tag{23}$$

Using the relation (20) and $c = 1/2$, we can write $A_{c,\sigma}$ as

$$A_{1/2,\sigma} = \frac{a_{11}}{2} + \frac{a_{12}}{2}\sigma + \frac{a_{21}}{4} + \frac{a_{22}}{4}\sigma = \frac{a_{21}}{2}\sigma + \Big(\frac{a_{11}}{2} + \frac{a_{21}}{4}\Big).$$

From the first EF conditions (21), a_{11} and a_{21} are uniquely determined as follows.

$$a_{11} = \frac{6\big(-7+4\cosh(\frac{z}{2})+3\cosh(z)\big)}{z\big(4\sinh(\frac{z}{2})+\sinh(z)\big)}, \tag{24}$$
$$a_{21} = \frac{12\big(3-2\cosh(\frac{z}{2})-\cosh(z)\big)}{z\big(4\sinh(\frac{z}{2})+\sinh(z)\big)}. \tag{25}$$

Obviously they satisfy (23). Therefore, we can conclude that the EF conditions (21) and (22) are compatible if and only if $c = 1/2$, (24) and (25). Note that for the numerical computation, the following series expansions should be employed:

$$a_{11} = 4 - \frac{1}{16}z^2 + \frac{7}{5760}z^4 - \frac{113}{3870720}z^6 + \frac{79}{92897280}z^8 - \frac{229}{11678515200}z^{10}$$

$$+\frac{55067}{76517631590400}z^{12}+\cdots,$$
$$a_{21}=-3+\frac{1}{16}z^2-\frac{1}{640}z^4+\frac{17}{430080}z^6-\frac{31}{30965760}z^8+\frac{691}{27249868800}z^{10}$$
$$-\frac{5461}{8501959065600}z^{12}+\cdots.$$

It is clear that in the limit $z\to 0$ the standard fourth order EP method is reproduced.

The derived scheme has at least the accuracy of order two because it is symmetric. Moreover since the coefficients satisfy the conditions for order three

$$\int_0^1\int_0^1\int_0^1 B_\sigma A_{\sigma,\tau}A_{\sigma,\nu}\mathrm{d}\sigma\mathrm{d}\tau\mathrm{d}\nu=\frac{1}{3}+\mathcal{O}(z^2),$$
$$\int_0^1\int_0^1\int_0^1 B_\sigma A_{\sigma,\tau}A_{\tau,\nu}\mathrm{d}\sigma\mathrm{d}\tau\mathrm{d}\nu=\frac{1}{6}+\mathcal{O}(z^2),$$

the scheme has the accuracy of order four.

4 Numerical examples

In this section we present two numerical experiments that confirm the effectiveness of the EPEFcRK methods. Through some typical Hamiltonian problems, we compare the EPEFcRK methods with the standard EPcRK methods. Note that although in the previous section we considered $\mathcal{F}_1=\{\exp(\lambda t),\exp(-\lambda t)\}$, we can automatically obtain EF schemes for $\mathcal{F}_2=\{\cos(\omega t),\sin(\omega t)\}$ by substituting $\lambda=i\omega$. In the following examples, we consider problems where we know a suitable value of the parameter ω in advance. Of course, the choice of the parameter ω is one of the important issues in the use of EF methods. Several standard ways are summarized in [48, Section 6]. All the computations were done in the computation environment: 2 GHz Intel Core i7, 8 GB memory, OS X 10.8.2. We used MATLAB (R2013a). Nonlinear equations were solved by *fsolve* with tolerance 10^{-16}.

Example 1. We consider the Kepler two-body problem defined by the Hamiltonian

$$H(\boldsymbol{q},\boldsymbol{p})=\frac{1}{2}\big(p_1^2+p_2^2\big)-\frac{1}{\sqrt{q_1^2+q_2^2}},$$

with the initial conditions $q_1=1-e$, $q_2=0$, $p_1=0$, $p_2=\sqrt{(1+e)/(1-e)}$, where e $(0\le e\le 1)$ represents the eccentricity of the elliptic orbit. This problem describes the motion of two bodies which attract each other. By placing the first body in the origin, (q_1,q_2) and (p_1,p_2) describe the position and velocity of the other body, respectively. The exact solution of this initial value problem is a 2π-periodic elliptic orbit in the (q_1,q_2)-plane with the eccentricity e. In the numerical experiments, we have chosen the values $e=0.02$, $\lambda=i\omega$ with $\omega=(q_1^2+q_2^2)^{-3/2}$.

Before showing the numerical results, we mention some implementation issues. For energy-preserving methods, we have to exactly compute the average of the vector field, i.e., the right hand side of (13) and (14) before the implementation. Although we can integrate them exactly for second order schemes, we cannot do that for fourth order ones. Instead, we have integrated them numerically, using *quad* with tolerance 10^{-10}. Obviously, the computational costs largely depend on not only the tolerance of *fsolve* but also that of *quad*. In the next example, this kind of problem does not occur.

The variations of the error of the Hamiltonian are shown in Fig. 1. All schemes preserve the Hamiltonian well. The reason why the accuracy of the fourth order schemes fall behind that of the second order schemes might be due to the tolerance of *quad*. In Fig. 2 (left) one can see that the errors are growing linearly with time for all four schemes. The result by the second order EPEFcRK scheme is more or less the same as that by the standard second order EPcRK scheme. But the result by the fourth order EPEFcRK scheme is better than that by the standard fourth order EPcRK scheme. Fig. 2 (right) shows the convergence of the numerical solutions. One can observe the expected convergence rates in all of the schemes.

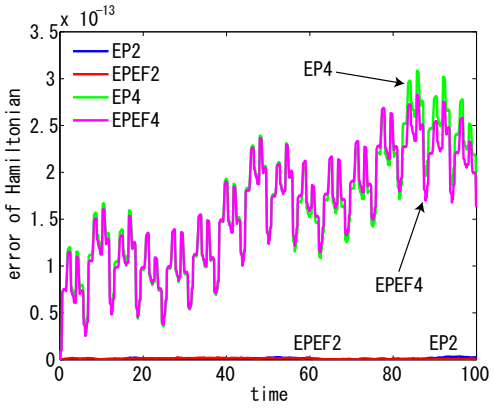

Figure 1: The variation of the error of Hamiltonian for Example 1 ($e = 0.02$). The step size was set to $h = 0.1$.

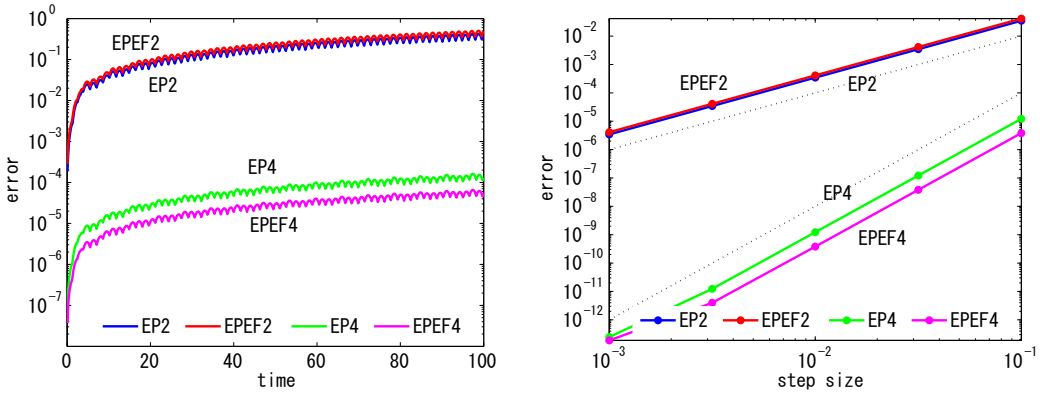

Figure 2: Left: The variation of the maximum global error for Example 1 ($e = 0.02$). The step size was set to $h = 0.1$. Right: The maximum global error at $t = 5$ for Example 1. The dashed lines have slopes two and four.

In general, the computational cost per step of high order schemes is large compared with that of low order schemes. In addition, in our situation, the effect of *quad* for fourth order schemes on the computational cost is not negligible. In order to objectively evaluate these effects we present in Fig. 3 the error versus CPU time, which indicates that the fourth order EPEFcRK scheme is the best in all four schemes.

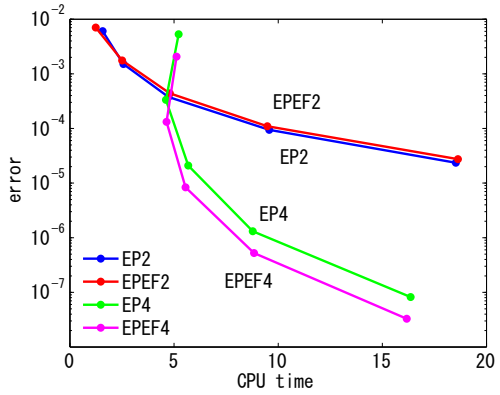

Figure 3: The error versus CPU-time at $t = 5$ for Example 1. For second order methods, the dots indicate the step length starting from the *left-side* with $h = 0.1/2$ and proceeding with $h = 0.1/2^m$, $m = 2, 3, \ldots$. For fourth order methods, the dots indicate the step length starting from the *top-side* with $h = 1/2$ and proceeding with $h = 1/2^m$, $m = 2, 3, \ldots$.

Example 2. We consider a cubic oscillatory Hamiltonian problem defined by

$$H(q,p) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 - \frac{1}{4}q^4.$$

with $\omega = 10$ and the initial condition $(q,p) = (1.5, 0)$.

The variations of the error of the Hamiltonian are shown in Fig. 4 (left). All schemes preserve the Hamiltonian well. Apparently, the error of fourth order EPEFcRK scheme seems to grow linearly. But we observed that this error is bounded and the error is more or less the same as those of other schemes (see Fig. 4 (right)).

In Fig. 5 (left) one can see that the errors are growing linearly with time for all four schemes. The results by the EPEFcRK schemes are better than those by the standard EPcRK schemes. Fig. 5 (right) shows the convergence of the numerical solutions. One can observe the expected convergence rates in all of the schemes.

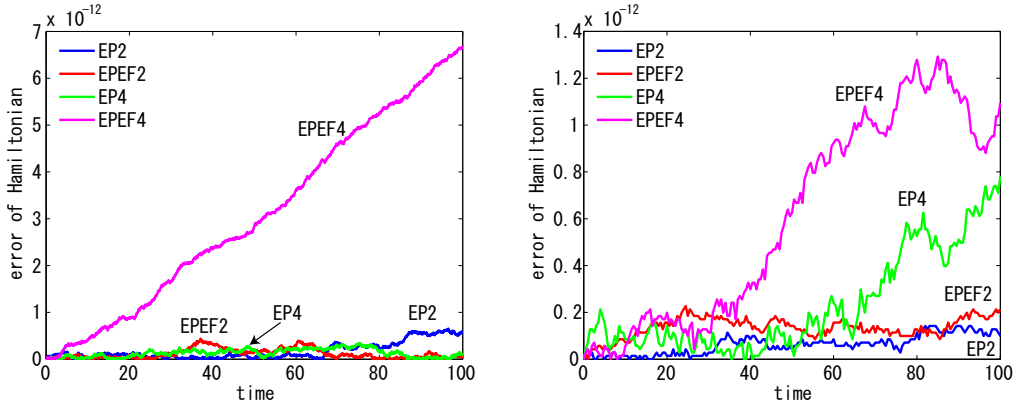

Figure 4: The variation of the error of Hamiltonian for Example 2. Left: The step size was set to $h = 0.05$. Right: The step size was set to $h = 0.5$.

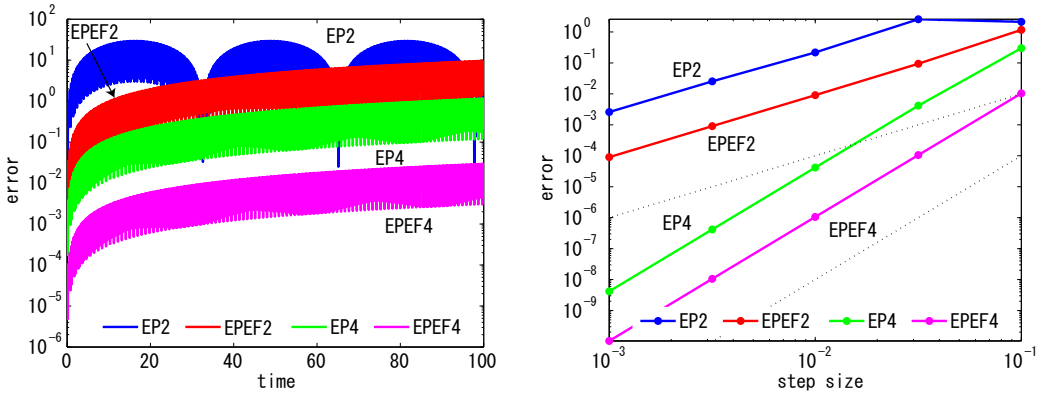

Figure 5: Left: The variation of the maximum global error for Example 2. The step size was set to $h = 0.05$. Right: The maximum global error at $t = 10$ for Example 2.

5 Discussions and conclusions

In this paper, we proved the conditions of energy-preservation in terms of the cRK methods, and developed the theory of standard EFcRK methods. Then based on the theories we constructed second and fourth order energy-preserving EFcRK (EPEFcRK) schemes. Through the numerical experiments for the problems with periodic or oscillatory solutions, we observed that the derived schemes in fact gave better numerical solutions than the standard energy-preserving schemes.

At this point, there naturally arises a question: is it possible to construct EPEF methods for Poisson systems? We give a short comment on this topic in Section 5.1. After that we discuss some future works in Section 5.2.

5.1 Extension to Poisson systems

We consider Poisson (non-canonical Hamiltonian) systems of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}y = B(y)\nabla H(y),$$

where $B(y)$ is a skew-symmetric matrix. For Poisson systems, the Hamiltonian $H(y(t))$ is also constant along the solution. The simplest example of energy-preserving methods for Poisson systems is

$$y_1 = y_0 + hB\left(\frac{y_0+y_1}{2}\right)\int_0^1 \nabla H((1-\tau)y_0 + \tau y_1)\mathrm{d}\tau$$

which reduces to the AVF integrator (12) when $B(y)$ is a constant matrix. The biggest difference between energy-preserving integrators for Hamiltonian and Poisson systems is that the latter treats the factors $B(y)$ and $\nabla H(y)$ differently. High-order energy-preserving method for Poisson systems was constructed by Cohen–Hairer [15], where the authors extended the energy-preserving cRK method [30] to a kind of partitioned methods.

We consider the following partitioned cRK method for Poisson systems defined by

$$Y_\tau = y_0 + h\sum_{j=1}^{s}\int_0^1 A^j_{\tau,\sigma}B(Y_j)\nabla H(Y_\sigma), \tag{26}$$

$$y_1 = y_0 + h \sum_{j=1}^{s} \int_0^1 B_\sigma^j B(Y_j) \nabla H(Y_\sigma), \tag{27}$$

where $B_\sigma^j = A_{1,\sigma}^j$. The conditions of energy-preservation are shown in the following theorem.

Theorem 5.1. A partitioned cRK method solving Poisson systems is energy-preserving if $\frac{\mathrm{d}}{\mathrm{d}\tau} A_{\tau,\sigma}^j$ is symmetric for each j.

Proof. The proof is similar to that of Theorem 3.1. □

We can develop EPEF methods based on this theorem, but we omit concrete examples because the procedure is similar to that illustrated in Section 3.

5.2 Future works

Our future works include the following.

- In this paper, we derive only second and fourth order EPEFcRK schemes. Higher order EPEFcRK schemes and more general framework for Hamiltonian and Poisson systems should be constructed. One of the difficulties there is that as far as we consider only the conditions of energy-preservation, symmetry and exponential-fitting, the problem is essentially underdetermined. There we have to consider order conditions as well.
- It would also be interesting to consider EPEF methods based on other generalization of the AVF method such as the Hamiltonian boundary value method [5, 6].
- In general, it is of interest to study whether numerical methods, especially energy-preserving methods, are conjugate symplectic and thus have the same long-time behaviour as symplectic methods. For standard energy-preserving methods (EPcRK methods), this point was already discussed in [32, 33], based on the fact that the energy-preserving methods can be expressed as B-series integrators. Similar discussions should be done for EPEFcRK methods. However, since EF methods are not B-series methods in general, we cannot directly apply the theory in [32, 33] to EPEFcRK methods.

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