Three-stage two-parameter symplectic, symmetric exponentially-fitted Runge-Kutta methods of Gauss type

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Abstract. We construct an exponentially-fitted variant of the well-known three stage Runge-Kutta method of Gauss-type. The new method is symmetric and symplectic by construction and it contains two parameters, which can be tuned to the problem at hand. Some numerical experiments are given.

Keywords: Symplectic methods; Exponential fitting
PACS: 02.60.Lj

INTRODUCTION

The study of methods for the numerical integration of ODEs which have periodic or oscillating solutions has lead to the development of so-called trigonometrically-fitted (or exponentially-fitted) methods. The aim of this approach is to derive more accurate and/or efficient algorithms than the general purpose ones by using the available information on the solutions. A detailed survey including an extensive bibliography on the subject of exponential-fitting can be found in [1].

On the other hand, oscillatory problems arise in different fields of applied sciences, and in may cases they are Hamiltonian systems. It has been widely recognized by several authors that symplectic integrators have some advantages for the preservation of qualitative properties of the flow over the standard integrators when they are applied to Hamiltonian systems. For the class of oscillatory Hamiltonian systems, in addition to using EF methods, it may be appropriate to consider symplectic methods that preserve the structure of the original flow. In addition, symmetric methods show a better long time behaviour than non symmetric ones when applied to reversible differential systems, as it is the case for conservative mechanical systems. In general, it has been proved that for all differential systems for which the flow is reversible, the numerical flow of a RK method will also be reversible iff (for a reversing symmetry that is linear or affine) it is symmetric [2]. An excellent overview of all this can be found in [3].

In this paper, we focus our attention on symmetric, symplectic, exponentially-fitted Runge-Kutta (EFRK) methods of Gauss type, and in particular we will consider the construction of a three stage method. Several authors have already studied methods of this type : Van de Vyver [4] first constructed an EF two-stage method starting from a so-called modified Runge-Kutta method, i.e. a method in which each internal stage contains an extra parameter γ_i. Later, Vanden Berghe and Van Daele [8, 9, 10] followed this approach to construct three-stage and four-stage EF methods of this type. The coefficients of their EF methods are selected such that both the internal stages and the final stage integrate exactly a set $\mathscr{S}$ of linearly independent functions. In [8, 9, 10] both $\mathscr{S}_{int}$ and $\mathscr{S}_{fin}$ take the form

$$\mathscr{S}^{(1)}_{K,P}(\mu) = \{1, t, t^2, \dots, t^K\} \cup \{\exp(\pm\mu t), t\exp(\pm\mu t), \dots, t^P \exp(\pm\mu t)\}\,. \qquad (1)$$

which is the same choice as in [1]. On the other hand, Calvo et al. [5, 6, 7] have considered three-stage methods with fixed and variable nodes for which S_{int} and S_{fin} take the form

$$\mathscr{S}^{(2)}_{K,P}(\mu) = \{1, t, t^2, \dots, t^K\} \cup \{\exp(\pm\mu t), \exp(\pm 2\mu t), \dots, \exp(\pm(P+1)\mu t)\}\,.$$

In this paper, following the approach used in [11], we consider the construction of a member of a class of methods that covers both cases, by starting from the general form

$$\widehat{\mathscr{S}}_{K,P}(\mu_0, \mu_1, \dots, \mu_P) = \{1, t, t^2, \dots, t^K\} \cup \{\exp(\pm\mu_0 t), \exp(\pm\mu_1 t), \dots, \exp(\pm\mu_P t)\}\,,$$

where the parameters μ_q, $q = 0, \dots, P$ are either real or appear as complex conjugate pairs. Clearly, if $\mu_0 = \mu_1/2 = \mu_2/3 = \dots = \mu_P/(P+1)$, this leads to the approach of Calvo and co-workers, while the approach of Vanden Berghe and co-workers is obtained when $\mu_0 = \mu_1 = \ldots = \mu_P$. The case that is discussed here in detail is a three-stage method, that contains two parameters μ_0 and μ_1.

THREE-STAGE TWO-PARAMETER METHODS

A symmetric, symplectic 3-stage Runge-Kutta method has the form

$$\begin{array}{c|ccc} \frac{1}{2}-\theta & \frac{b_1}{2} & \frac{b_2}{2}-\alpha_2 & \frac{b_1}{2}-\alpha_3 \\ \frac{1}{2} & \frac{b_1}{2}-\alpha_4 & \frac{b_2}{2} & \frac{b_1}{2}+\alpha_4 \\ \frac{1}{2}+\theta & \frac{b_1}{2}+\alpha_3 & \frac{b_2}{2}+\alpha_2 & \frac{b_1}{2} \\ \hline & b_1 & b_2 & b_1 \end{array}$$

whereby symplecticity requires that $b_1\,\alpha_2 + b_2\,\alpha_4 = 0$. We consider the construction of a method for which

$$\mathscr{S}_{int} = \{1, \exp(\mu_0\,x), \exp(-\mu_0\,x)\} \quad \text{and} \quad \mathscr{S}_{fin} = \{1, \exp(\mu_0\,x), \exp(-\mu_0\,x), \exp(\mu_1\,x), \exp(-\mu_1\,x)\}\,.$$

Therefore, we proceed in two steps. Firstly, we impose

$$\mathscr{S}_{int} = \{1, \exp(\mu_0\,x), \exp(-\mu_0\,x)\} \subset \mathscr{S}_{fin}$$

which allows us to express all parameters b_1, b_2, α_2, α_3 in terms of θ. One then finds that b_1 can be written as

$$b_1 = G(z_0, 2\,z_0)\,, \qquad z_0 := \mu_0\,h\,, \qquad G(a,b) := \frac{\frac{\sinh(a/2)}{a/2} - \frac{\sinh(b/2)}{b/2}}{\cosh(a\,\theta) - \cosh(b\,\theta)}\,. \tag{2}$$

In fact the method that is obtained in this way is the one that was already reported by Calvo et al. in [5], formulas (26) and (27), imposing

$$\mathscr{S}_{int} = \{1, \exp(\mu_0\,x), \exp(-\mu_0\,x)\} \qquad \textit{and} \qquad \mathscr{S}_{fin} = \{1, \exp(\mu_0\,x), \exp(-\mu_0\,x), \exp(2\,\mu_0\,x), \exp(-2\,\mu_0\,x)\}\,,$$

i.e. by accident the functions $\exp(\pm 2\,\mu_0\,x)$ are integrated exactly by the final stage. Next we impose $\{\exp(\mu_1\,x), \exp(-\mu_1\,x)\} \subset \mathscr{S}_{fin}$, and this leads to $b_1 = G(z_0, z_1)$ with $z_1 := \mu_1\,h$. It is thus clear that we obtain the relation $G(z_0, z_1) = G(z_0, 2\,z_0)$ from which θ can be determined. In general, an iterative procedure is needed to determine θ, but some special cases allow an explicit computation of θ. For instance, if $z_1 = 3\,z_0$ the 3-stage method of Calvo et al. [5] with variable knots is obtained and in that case, θ is given by formula (32) of [5], or by the equivalent formula $\theta = \frac{1}{z_0}\text{arccosh}(\beta)$ with

$$\beta = \frac{1}{6}\left(2\,\cosh(z_0/2) - 1 + \sqrt{4\,\cosh^2(z_0/2) + 8\,\cosh(z_0/2) + 13}\right)\,.$$

For small values of $|z|$ and $|z_1|$ (say smaller than 0.1), the use of a Taylor series (also for the computation of the coefficients of the RK method) is to be preferred. Then θ can be written as

$$\begin{aligned}\theta = {} & \frac{\sqrt{15}}{10} + \frac{\sqrt{15}}{21000}\left(5\,z_0^2 + z_1^2\right) - \frac{\sqrt{15}}{1058400000}\left(2295\,z_0^4 + 85\,z_0^2\,z_1^2 + 131\,z_1^4\right) \\ & + \frac{\sqrt{15}}{9779616\,10^7}\left(1730250\,z_0^6 - 1653665\,z_0^4\,z_1^2 - 5765\,z_0^2\,z_1^4 + 26974\,z_1^6\right) \\ & - \frac{\sqrt{15}}{32038022016\,10^8}\left(315442125\,z_0^8 - 1150951980\,z_0^6\,z_1^2 - 223250821\,z_0^4\,z_1^4 + 430340\,z_0^2\,z_1^6 + 1175117\,z_1^8\right) \\ & + \ldots\end{aligned}$$

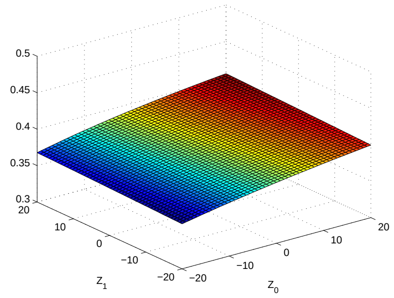

FIGURE 1. Plot of θ as a function of Z_0 and Z_1.

Special care is also needed in case $z_1 \approx z_0$ or $z_1 \approx 2z_0$. In the particular case that $z_1 = z_0$, l'Hopital's rule learns that θ follows from

$$\lim_{z_1 \to z_0} G(z_0, z_1) = \frac{\cosh(z_0/2) - \frac{\sinh(z_0/2)}{z_0/2}}{z_0\,\theta\,\sinh(z_0\,\theta)} = G(z_0, 2z_0)\,.$$

Similarly, it is found that in case $z_1 = 2z_0$, θ follows from

$$\lim_{z_1 \to 2z_0} G(2z_0, z_1) = \frac{\cosh(z_0) - \frac{\sinh(z_0)}{z_0}}{2z_0\,\theta\,\sinh(2z_0\,\theta)} = G(z_0, 2z_0)\,.$$

It should be noted that, for computational purposes, all formula can best be written down in terms of the functions η and ξ of Ixaru [1], p. 64, which are defined as $\xi(Z) = \cos(i\sqrt{Z})$ and $\eta(Z) = \sin(i\sqrt{Z})/(i\sqrt{Z})$ if $Z \neq 0$ and $\eta(0) = 1$. This formalism allows to handle both the exponential (Z>0) and the trigonometric case (Z<0) and the coefficients of the methods can be expressed quite easily in this setting.

The behaviour of θ as a function of $Z_0 := z_0^2$ and $Z_1 := z_1^2$ for $-20 \leq Z_0, Z_1 \leq 20$ is shown in Figure 1.

SOME NUMERICAL RESULTS

Finally, we present some numerical experiments to test the behaviour of the new two-parameter EFRK method derived in this paper. We compare our results with the classical Gauss method and the 3 stage EF method of Calvo (both fixed and variable nodes). All methods are symplectic, symmetric and the global preservation of symplecticness only holds for a fixed step-size together with fixed fitting frequencies along the integration.

The first problem we consider is the well-known Kepler problem [4], for which the Hamiltonian can be written as

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

The initial conditions are chosen such that at $t = 0 : (q_1, q_2, p_1, p_2) = \left(1 - e, 0, 0, \sqrt{\frac{1+e}{1-e}}\right)$ whereby $e = 0.001$. To integrate the problem numerically, we follow [4, 5, 9] and put $z_0 = \mathrm{i}\,(q_1^2 + q_2^2)^{-3/2}\,h$, which is almost constant. For our two-parameter scheme, we have put $z_1 = z_0/2$.

The second problem we consider is a perturbed Kepler problem [5, 9] with

$$H(p,q) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \frac{1}{\sqrt{q_1^2 + q_2^2}} - \frac{2\varepsilon + \varepsilon^2}{3\sqrt{(q_1^2 + q_2^2)^3}}$$

whereby $\varepsilon = 0.001$ and initial conditions such that $t = 0 : (q_1, q_2, p_1, p_2) = (1, 0, 0, 1 + \varepsilon)$. For the numerical integration, we have put $z_0 = \mathrm{i}\,h$ and $z_1 = z_0/2$.

We have integrated both problems in $[0, 1000]$ with fixed stepsize $h = 2^{-m}$, $m = 1, \ldots, 3$ and we computed the maximum error over the integration interval. The results are shown in Figure 2.

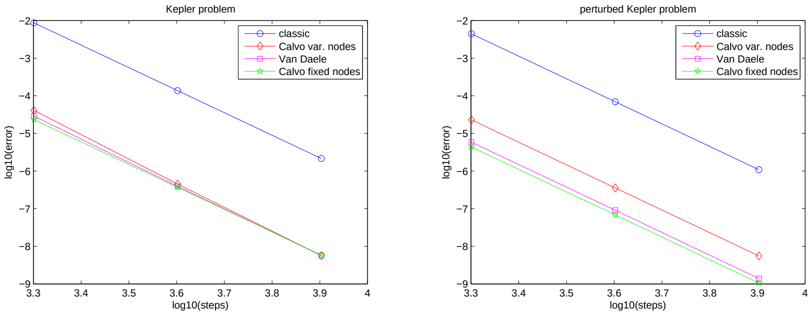

FIGURE 2. Maximum errors over the integration interval for the Kepler problem (left) and the perturbed Kepler problem (right) as a function of the number of steps.

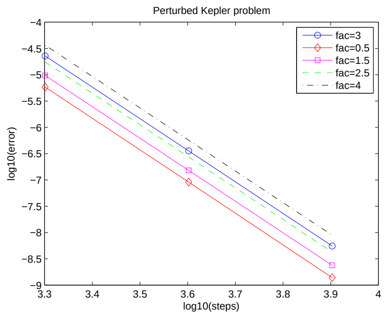

FIGURE 3. Maximum errors over the integration interval for the perturbed Kepler problem as a function of the number of steps for various values of fac where $z_1 = \mathrm{fac}\, z_0$.

The efficiency and accuracy that can be obtained by EF methods of course strongly depend upon the choice of the μ-parameters. How their values should be chosen is still an open question. The value that was chosen for z_0 was the same as the one that was chosen by the other cited authors. For the two-parameter method, the choice $z_1 = z_0/2$ was made. In Figure 3 the results are shown for some other choices of z_1.

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