

Exponentially fitted symplectic integrator

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In this paper a procedure for constructing efficient symplectic integrators for Hamiltonian problems is introduced. This procedure is based on the combination of the exponential fitting technique and symplecticness conditions. Based on this procedure, a simple modified Runge-Kutta-Nyström second-order algebraic exponentially fitted method is developed. We give explicitly the symplecticness conditions for the modified Runge-Kutta-Nyström method. We also give the exponential fitting and trigonometric fitting conditions. Numerical results indicate that the present method is much more efficient than the “classical” symplectic Runge-Kutta-Nyström second-order algebraic method introduced by M.P. Calvo and J.M. Sanz-Serna [J. Sci. Comput. (USA) **14**, 1237 (1993)]. We note that the present procedure is appropriate for all near-unimodal systems.

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I. INTRODUCTION

Hamiltonian systems of ordinary differential equations can be found in many areas of mechanics, physics, optics, chemistry, and elsewhere [2]. Hamiltonian systems of ordinary differential equations can be written as

$$\dot{p}^s = -\frac{\partial H}{\partial q^s}, \quad \dot{q}^s = \frac{\partial H}{\partial p^s}, \quad 1 \leq s \leq DF, \quad (1)$$

where s denotes the number of degrees of freedom. We note here that $H = H(\mathbf{p}, \mathbf{q})$ is a sufficiently smooth and real function of $2s$ real variables. We also note that the dot denotes differentiation with respect to time (from now on, the time will be represented by t).

During the last decades, many symplectic or canonical integrators have been developed for the numerical solution of the problem (1) (see Refs. [3,4] and references therein).

When a one-step numerical method (which uses a constant step size h) is used for the approximate solution of the above problem, a transformation in phase space $\phi_h(\mathbf{p}_0, \mathbf{q}_0)$ is defined. This space approximates the solution with a step size equal to h starting from the initial point $(\mathbf{p}_0, \mathbf{q}_0)$. When classical one-step methods, such as explicit Runge-Kutta methods, are used for the integration of Hamiltonian problems, the above transformation is nonsymplectic (see Ref. [5]).

In recent years, much research has been done on exponential-type methods. This is because these methods

have very good properties when applied to the solution of oscillating problems (see, for instance, Refs. [6–11]).

In this paper we introduce a procedure for constructing efficient symplectic integrators for Hamiltonian problems. This procedure is based on the combination of the exponential fitting technique and symplecticness conditions. We develop a simple modified Runge-Kutta-Nyström second-order algebraic exponentially fitted method based on the above procedure. In Sec. II we present the modified Runge-Kutta-Nyström method and we give its symplecticness conditions. In Sec. III we present the conditions that are necessary in order that the method integrates exactly any linear combination of exponential functions, and we construct the exponential fitting Runge-Kutta-Nyström method. In Sec. IV we present the conditions that are necessary in order that the method integrates exactly a single harmonic oscillator, and we construct the trigonometric fitting Runge-Kutta-Nyström method. In Sec. V we present some numerical results for periodic and oscillatory problems. Finally, conclusions are presented.

II. SYMPLECTIC MODIFIED RUNGE-KUTTA-NYSTRÖM METHOD

For the numerical solution of the problem,

$$\mathbf{q}'' = \mathbf{f}(\mathbf{q}), \quad (2)$$

consider the following m -stage modified Runge-Kutta-Nyström method (see, for details, Ref. [13]):

$$\mathbf{q}_n = g_1 \mathbf{q}_{n-1} + h g_2 \dot{\mathbf{q}}_{n-1} + h^2 \sum_{j=0}^m \beta_j f_j, \quad (3)$$

$$\dot{\mathbf{q}}_n = g_3 \dot{\mathbf{q}}_{n-1} + h \sum_{j=0}^m b_j f_j, \quad (4)$$

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where

$$f_i = f \left(\mathbf{q}_{n-1} + h \gamma_i \dot{\mathbf{q}}_{n-1} + h^2 \sum_{j=0}^{i-1} a_{i,j} f_j \right), \quad i=0(1)m, \tag{5}$$

and a, b , and β are smooth functions depending on the product of the frequency ν and the step size h , and $\gamma_0=0$ and $\gamma_m=1$.

If we transform the problem (2) into the system of first-order equations,

$$\mathbf{p}' = \mathbf{f}(\mathbf{q}), \quad \mathbf{q}' = \mathbf{p}, \tag{6}$$

then the above method (4),(5) can be written as

$$\mathbf{q}_n = g_1 \mathbf{q}_{n-1} + h g_2 \mathbf{p}_{n-1} + h^2 \sum_{j=0}^i \beta_j f_j, \tag{7}$$

$$\mathbf{p}_n = g_3 \mathbf{p}_{n-1} + h \sum_{j=0}^m b_j f_j, \tag{8}$$

where

$$f_i = f \left(\mathbf{q}_{n-1} + h \gamma_i \mathbf{p}_{n-1} + h^2 \sum_{j=0}^{i-1} a_{i,j} f_j \right) \tag{9}$$

and $\gamma_0=0$ and $\gamma_m=1$.

In this paper we restrict our attention to the simplest of the above method, i.e., we investigate the case $m=1$.

It is known (for more details see Refs. [4] and [5]) that the symplecticness conditions come from the requirement

$$d\mathbf{p}_{n+1} \wedge d\mathbf{q}_{n+1} = d\mathbf{p}_n \wedge d\mathbf{q}_n. \tag{10}$$

We note here that the proposed map $(p_n, q_n) \rightarrow (p_{n+1}, q_{n+1})$ is volume preserving if Eq. (10) holds.

For example, for case $m=1$, and based on the above formula, the following symplecticness conditions are obtained for the modified Runge-Kutta-Nyström method (8),(9):

$$\begin{aligned} g_1 g_3 &= 1, \\ \beta_0 g_3 - b_0 g_2 &= 0, \\ \beta_1 g_3 - b_1 g_2 + g_1 b_1 \gamma_1 &= 0, \\ \beta_1 b_0 - b_1 \beta_0 + g_1 b_1 a_{1,0} &= 0. \end{aligned} \tag{11}$$

We also note here that for the above Runge-Kutta-Nyström method we make use of the well-known simplifying assumptions [14],

$$\sum_{j=0}^{i-1} a_{i,j} = \frac{\gamma_i^2}{2}, \quad 1 \leq i \leq m. \tag{12}$$

III. EXPONENTIAL FITTING MODIFIED SYMPLECTIC RUNGE-KUTTA-NYSTRÖM METHOD

Requiring the above modified Runge-Kutta-Nyström method to integrate exactly the exponential function $\exp(\pm \nu x)$ we have the following equations:

$$\exp(w) = g_1 + g_2 w + (\beta_0 + \beta_1) w^2 + \beta_1 \gamma_1 w^3 + \beta_1 a_{1,0} w^4, \tag{13}$$

$$\exp(w) = g_3 + (b_0 + b_1) w + b_1 \gamma_1 w^2 + b_1 a_{1,0} w^3, \tag{14}$$

where

$$w = \nu h.$$

Assuming that

$$\gamma_1 = 1, \quad g_3 = 1 \tag{15}$$

and solving the system of equations (11), (13), and (14) the following coefficients for the modified exponential fitting symplectic Runge-Kutta-Nyström method are obtained:

$$\begin{aligned} g_1 &= 1, \quad b_0 = \frac{1}{2}, \\ g_2 &= -\frac{1}{2} \frac{w^2 + (2w+2)[1 - \exp(w)]}{w \exp(w)}, \\ b_1 &= -\frac{w + 2[1 - \exp(w)]}{w(2 + 2w + w^2)}, \\ \beta_0 &= -\frac{1}{4} \frac{w^2 + (2w+2)[1 - \exp(w)]}{w \exp(w)}, \\ \beta_1 &= \frac{1}{2} \frac{[2 + w - 2 \exp(w)] S(w)}{w(2 + 2w + w^2) \exp(w)}, \end{aligned} \tag{16}$$

where

$$S(w) = w^2 - 2 \exp(w) + 2w + 2.$$

For small values of v , the above formulas are subject to heavy cancellations. In this case, the following Taylor series expansions must be used:

$$\begin{aligned}
 g_2 &= 1 + \frac{1}{6}w^2 - \frac{1}{8}w^3 + \frac{1}{20}w^4 - \frac{1}{72}w^5 + \frac{1}{336}w^6 - \frac{1}{1920}w^7 \\
 &\quad + \frac{1}{12\,960}w^8 - \frac{1}{100\,800}w^9 + \frac{1}{887\,040}w^{10} \\
 &\quad - \frac{1}{8\,709\,120}w^{11} + \frac{1}{94\,348\,800}w^{12} - \frac{1}{1\,117\,670\,400}w^{13} \\
 &\quad + \frac{1}{14\,370\,048\,000}w^{14} + \dots, \\
 b_1 &= \frac{1}{2} - \frac{1}{12}w^2 + \frac{1}{8}w^3 - \frac{3}{40}w^4 + \frac{1}{72}w^5 + \frac{1}{42}w^6 - \frac{59}{1920}w^7 \\
 &\quad + \frac{61}{3240}w^8 - \frac{349}{100\,800}w^9 - \frac{5279}{887\,040}w^{10} + \frac{66\,907}{8\,709\,120}w^{11} \\
 &\quad - \frac{444\,079}{94\,348\,800}w^{12} + \frac{967\,429}{1\,117\,670\,400}w^{13} \\
 &\quad + \frac{21\,379\,951}{14\,370\,048\,000}w^{14} + \dots, \\
 \beta_0 &= \frac{1}{2} + \frac{1}{12}w^2 - \frac{1}{16}w^3 + \frac{1}{40}w^4 - \frac{1}{144}w^5 + \frac{1}{672}w^6 \\
 &\quad - \frac{1}{3840}w^7 + \frac{1}{25\,920}w^8 - \frac{1}{201\,600}w^9 + \frac{1}{1\,774\,080}w^{10} \\
 &\quad - \frac{1}{17\,418\,240}w^{11} + \frac{1}{188\,697\,600}w^{12} \\
 &\quad - \frac{1}{2\,235\,340\,800}w^{13} + \frac{1}{28\,740\,096\,000}w^{14} + \dots, \\
 \beta_1 &= \frac{1}{12}w^2 - \frac{1}{16}w^3 + \frac{1}{90}w^4 + \frac{7}{288}w^5 - \frac{69}{2240}w^6 + \frac{217}{11\,520}w^7 \\
 &\quad - \frac{1571}{453\,600}w^8 - \frac{4799}{806\,400}w^9 + \frac{91\,997}{11\,975\,040}w^{10} \\
 &\quad - \frac{409\,919}{87\,091\,200}w^{11} + \frac{65\,503}{75\,675\,600}w^{12} + \frac{19\,954\,621}{13\,412\,044\,800}w^{13} \\
 &\quad - \frac{2\,870\,310\,293}{1\,494\,484\,992\,000}w^{14} + \dots. \tag{17}
 \end{aligned}$$

We note here that in the cases when w is allowed to be complex and the denominator,

$$p(w) = w(2 + 2w + w^2)\exp(w), \tag{18}$$

is equal to zero, the procedure described below is followed.

Denote by w_k , for $k = -1, 1$, the zeros of Eq. (18). [Set $w_0 = 0$, although w_0 is not a root of $p(w)$. w_0 is, in fact a removable singularity for the coefficients as functions of w .]

If $w = w_k$, use the coefficients of the classical method of Calvo and Sanz-Serna.

If $w \neq w_k$ for any k and $p(w)$ is not close to 0 then use Eq. (16).

If $w \neq w_k$ but $p(w)$ is close to 0, then Eq. (16) cannot be used as given because the coefficients are ill conditioned. Instead, find the two poles $w_k < w_{k+1}$ such that $w_k < w < w_{k+1}$, expand the coefficients in Euler-MacLaurin series

$$\sum_{i=0}^{\infty} a_i (w - \bar{w})^i,$$

where $\bar{w} = (w_k + w_{k+1})/2$, and use truncated MacLaurin expansions instead of the Taylor expansion at the origin (which need not converge). Such a MacLaurin expansion converge with radius $\rho = (w_{k+1} - w_k)/2$.

IV. TRIGONOMETRIC FITTING MODIFIED SYMPLECTIC RUNGE-KUTTA-NYSTRÖM METHOD

Requiring the above modified Runge-Kutta-Nyström method to integrate exactly the differential equation $d^2 y/dt^2 = -v^2 y$, we have the following equations

$$\begin{aligned}
 \cos(w) &= g_1 - (\beta_0 + \beta_1)w^2 + \beta_1 a_{1,0} w^4, \\
 \sin(w) &= g_2 w - \beta_1 a_{1,0} w^3, \\
 -\sin(w) &= -(b_0 + b_1)w + b_1 a_{1,0} w^3, \\
 \cos(w) &= g_3 - b_1 \gamma_1 w^2, \tag{19}
 \end{aligned}$$

where

$$w = v h.$$

Assuming that

$$\gamma_1 = 1 \tag{20}$$

and solving the system of equations (11),(19) the following coefficients for the modified trigonometric fitting symplectic Runge-Kutta-Nyström method are obtained:

$$\begin{aligned}
 g_1 &= -\frac{2}{w^2 \cos(w) - 2 \cos(w) - 2w \sin(w)}, \\
 g_2 &= \frac{1}{4} \frac{T_0}{w [w^2 \cos(w) - 2 \cos(w) - 2w \sin(w)]}, \\
 g_3 &= \cos(w) + w \sin(w) - \frac{1}{2} \cos(w) w^2,
 \end{aligned}$$

$$b_1 = \frac{1}{w} \left(\sin(w) - \frac{1}{2} w \cos(w) \right),$$

$$b_0 = -\frac{1}{4} [w^2 \cos(w) - 2 \cos(w) - 2w \sin(w)],$$

$$\beta_0 = \frac{T_1}{8wT_2},$$

$$\beta_1 = \frac{1}{4} \frac{T_3 + 6w \sin(2w) - w^3 \sin(2w)}{w^2[w^2 \cos(w) - 2 \cos(w) - 2w \sin(w)]}, \quad (21)$$

where

$$T_0 = 8w[w \sin(2w) - 1 + \cos(2w)] - 4[\sin(2w) + w^3 \cos(2w)] - w^4 \sin(2w),$$

$$T_1 = 8[\cos(w) - \cos(3w)] + 4w[11 \sin(w) - 5 \sin(3w)] - 24w^2[\cos(w) - \cos(3w)] + 16w^3 \sin(3w) - 2w^4[\cos(w) + 3 \cos(3w)] - w^5[\sin(w) + \sin(3w)],$$

$$T_2 = -4w^2 \sin(2w) + w^3 \cos(2w) + w^4 + 4w \sin(2w) - 6w^2 \cos(2w) + 2w^2$$

and

$$T_3 = 4[\cos(2w) - 1 - w^2 \cos(2w)].$$

For small values of v the above formulas are subject to heavy cancellations. In this case the following Taylor series expansions must be used.

$$g_1 = 1 - \frac{1}{8}w^4 + \frac{1}{72}w^6 + \frac{29}{1920}w^8 - \frac{349}{100800}w^{10} - \frac{14197}{8709120}w^{12} + \frac{708709}{1117670400}w^{14} + \dots,$$

$$g_2 = 1 - \frac{1}{6}w^2 - \frac{3}{40}w^4 + \frac{11}{1008}w^6 + \frac{787}{51840}w^8 - \frac{15361}{4435200}w^{10} - \frac{922799}{566092800}w^{12} + \frac{63783803}{100590336000}w^{14} + \dots,$$

$$g_3 = 1 + \frac{1}{8}w^4 - \frac{1}{72}w^6 + \frac{1}{1920}w^8 - \frac{1}{100800}w^{10} + \frac{1}{8709120}w^{12} - \frac{1}{1117670400}w^{14} + \dots,$$

$$b_0 = \frac{1}{2} + \frac{1}{16}w^4 - \frac{1}{144}w^6 + \frac{1}{3840}w^8 - \frac{1}{201600}w^{10} + \frac{1}{17418240}w^{12} - \frac{1}{223534800}w^{14} + \dots,$$

$$b_1 = \frac{1}{2} + \frac{1}{12}w^2 - \frac{1}{80}w^4 + \frac{1}{2016}w^6 - \frac{1}{103680}w^8 + \frac{1}{8870400}w^{10} - \frac{1}{1132185600}w^{12} + \frac{1}{201180672000}w^{14} + \dots,$$

$$\beta_0 = \frac{1}{2} - \frac{1}{12}w^2 - \frac{3}{80}w^4 + \frac{11}{2016}w^6 + \frac{787}{103680}w^8 - \frac{15361}{8870400}w^{10} - \frac{922799}{1132185600}w^{12} + \frac{63783803}{201180672000}w^{14} + \dots,$$

$$\beta_1 = -\frac{1}{12}w^2 + \frac{1}{90}w^4 + \frac{17}{1120}w^6 - \frac{1571}{453600}w^8 - \frac{78083}{47900160}w^{10} + \frac{95971}{151351200}w^{12} + \frac{55282547}{373621248000}w^{14} + \dots \quad (22)$$

It can be seen that when $w \rightarrow 0$ the above method becomes the classical symplectic second-order algebraic Runge-Kutta-Nyström method mentioned in the paper of Calvo and Sanz-Serna [1].

We note here that in the cases when the denominator,

$$p(w) = (w^2 - 2)\cos(w) - 2w \sin(w), \quad (23)$$

is equal to zero the procedure described below is followed.

Denote by w_k , for $k = \dots, -2, -1, 1, 2, \dots$, the zeros of Eq. (23). [Set $w_0 = 0$, although w_0 is not a root of $p(w)$. w_0 is, in fact, a removable singularity for the coefficients as functions of w .]

If $w = w_k$, use the coefficients of the classical method of Calvo and Sanz-Serna.

If $w \neq w_k$ for any k and $p(w)$ is not close to 0 then use Eq. (21).

If $w \neq w_k$ but $p(w)$ is close to 0, then Eq. (21) cannot be used as given because the coefficients are ill conditioned. Instead, find the two poles $w_k < w_{k+1}$ such that $w_k < w < w_{k+1}$, expand the coefficients in Euler-MacLaurin series

$$\sum_{i=0}^{\infty} a_i(w - \bar{w})^i,$$

where $\bar{w} = (w_k + w_{k+1})/2$, and use truncated MacLaurin expansions instead of the Taylor expansion at the origin (which need not converge). Such a MacLaurin expansion converges with radius $\rho = (w_{k+1} - w_k)/2$.

TABLE I. Comparison of the absolute maximum error in the approximations obtained to the inhomogeneous problem using the classical second-order symplectic Runge-Kutta-Nyström method [1] [which is indicated as method (a)] and the trigonometrically fitted symplectic Runge-Kutta-Nyström one [which is indicated as method (b)]. The empty areas indicate that the error is greater than 1 (or overflow occurs).

Step size h	Method (a)	Method (b)
$\frac{1}{4}$		4.4×10^{-1}
$\frac{1}{8}$		1.3×10^{-1}
$\frac{1}{16}$		1.5×10^{-2}
$\frac{1}{32}$		2.2×10^{-3}
$\frac{1}{64}$		4.4×10^{-4}
$\frac{1}{128}$		1.0×10^{-4}
$\frac{1}{256}$		2.6×10^{-5}
$\frac{1}{512}$		6.6×10^{-6}
$\frac{1}{1024}$	2.8×10^{-1}	1.7×10^{-6}

V. NUMERICAL EXAMPLES FOR PERIODIC AND OSCILLATORY PROBLEMS

In this section we apply the symplectic Runge-Kutta-Nyström method to four problems. The first is an inhomogeneous problem, the second is the nonlinear undamped Duffing equation, the third is the “almost” periodic orbit problem studied by Stiefel and Bettis [12], and the fourth is Kepler’s problem.

A. Inhomogeneous equation

We consider the following problem

$$y'' = -100y + 99 \sin x, \quad y(0) = 1, \quad y'(0) = 11, \quad (24)$$

whose analytical solution is $y(x) = \cos 10x + \sin 10x + \sin x$.

Equation (24) has been solved numerically for $0 \leq x \leq 1000$ using the classical second-order algebraic symplectic Runge-Kutta-Nyström method [1] [which is indicated as method (a)] and the trigonometrically fitted symplectic Runge-Kutta-Nyström one [which is indicated as method (b)]. For this problem $v = 10$. In Table I we present the absolute maximum error which is equal to

$$\text{Abserr} = \max_{x=0}^{x=1000} |\text{Analyt}(x) - \text{Approx}(x)|, \quad (25)$$

where Abserr is the absolute maximum error, $\text{Analyt}(x)$ is the analytical solution, and $\text{Approx}(x)$ is the approximate solution.

TABLE II. Comparison of the absolute maximum error in the approximations obtained to the Duffing’s equation using the classical second-order symplectic Runge-Kutta-Nyström method [1] [which is indicated as method (a)] and the trigonometrically fitted symplectic Runge-Kutta-Nyström one [which is indicated as method (b)]. The empty areas indicate that the error is greater than 1 (or overflow occurs).

Step size h	Method (a)	Method (b)
2		3.9×10^{-1}
1		5.1×10^{-2}
$\frac{1}{2}$		5.0×10^{-3}
$\frac{1}{4}$	3.4×10^{-1}	5.6×10^{-4}
$\frac{1}{8}$	7.0×10^{-2}	6.8×10^{-5}
$\frac{1}{16}$	1.7×10^{-2}	8.7×10^{-6}
$\frac{1}{32}$	4.9×10^{-3}	1.2×10^{-6}
$\frac{1}{64}$	1.8×10^{-3}	2.0×10^{-7}
$\frac{1}{128}$	8.2×10^{-4}	3.9×10^{-8}

B. Duffing’s equation

We consider the nonlinear undamped Duffing equation,

$$y'' + y + y^3 = B \cos(\omega x), \quad (26)$$

where $B = 0.002$ and $\omega = 1.01$. The analytical solution of the above equation is given by

$$y(x) = \sum_{i=0}^3 A_{2i+1} \cos[(2i+1)\omega x], \quad (27)$$

where $A_1 = 0.200\ 179\ 477\ 536$, $A_3 = 0.24\ 694\ 614\ 310^{-3}$, $A_5 = 0.30\ 401\ 610^{-6}$, and $A_7 = 0.37\ 410^{-9}$.

Equation (26) has been solved numerically for $0 \leq x \leq 1000$ using the above mentioned methods with boundary conditions of the form

$$y(0) = A_1 + A_3 + A_5 + A_7, \quad y'(0) = 0, \quad (28)$$

where the A_i are given as above. For this problem $v = 1$. In Table II we present the absolute maximum error.

C. An orbit problem studied by Stiefel and Bettis

We consider the following “almost” periodic orbit problem studied by Stiefel and Bettis [12]:

$$z'' + z = 0.001e^{ix}, \quad z(0) = 1, \quad z'(0) = 0.9995i, \quad z \in C, \quad (29)$$

whose analytical solution is given by

$$z(x) = u(x) + iv(x), \quad u, v \in R,$$

$$u(x) = \cos x + 0.0005x \sin x,$$

TABLE III. Comparison of the absolute maximum error in the approximations obtained to the problem of Stiefel and Bettis using the classical second-order symplectic Runge-Kutta-Nyström method [1] [which is indicated as Method (a)] and the trigonometrically fitted symplectic Runge-Kutta-Nyström one [which is indicated as Method (b)]. The empty areas indicate that the error is greater than 1 (or overflow occurs).

Step size h	Method (a)	Method (b)
4		3.9×10^{-1}
2		8.2×10^{-2}
1		4.7×10^{-2}
$\frac{1}{2}$		1.1×10^{-2}
$\frac{1}{4}$		2.7×10^{-3}
$\frac{1}{8}$		6.5×10^{-4}
$\frac{1}{16}$	8.3×10^{-1}	1.6×10^{-4}
$\frac{1}{32}$	2.1×10^{-1}	4.1×10^{-5}
$\frac{1}{64}$	5.2×10^{-2}	1.0×10^{-5}
$\frac{1}{128}$	1.3×10^{-2}	2.5×10^{-6}

$$v(x) = \sin x - 0.0005x \cos x. \quad (30)$$

The solution (30) represents motion on a perturbation of a circular orbit in the complex plane.

We write Eq. (29) in the equivalent form

$$\begin{aligned} u'' + u &= 0.001 \cos x, & u(0) &= 1, & u'(0) &= 0, \\ v'' + v &= 0.001 \sin x, & v(0) &= 0, & v'(0) &= 0.9995. \end{aligned} \quad (31)$$

The equivalent system of equations (31) has been solved numerically for $0 \leq x \leq 1000$ using the above mentioned methods. For this problem $v = 1$. In Table III we present the absolute maximum error.

D. Kepler's problem

We consider the following system of coupled differential equations, which is well known as Kepler's problem:

$$\begin{aligned} y'' &= -\frac{y}{(y^2 + z^2)^{3/2}}, & z'' &= -\frac{z}{(y^2 + z^2)^{3/2}}, \\ y(0) &= 1, & y'(0) &= 0, & z(0) &= 0, & z'(0) &= 1, \end{aligned} \quad (32)$$

whose analytical solution is given by

$$y(x) = \cos(x), \quad z(x) = \sin(x). \quad (33)$$

The above system of equations (32) has been solved numerically for $0 \leq x \leq 1000$ using the above mentioned methods.

TABLE IV. Comparison of the absolute maximum error in the approximations obtained to the two-body problem using the classical second-order symplectic Runge-Kutta-Nyström method [1] [which is indicated as Method (a)] and the trigonometrically fitted symplectic Runge-Kutta-Nyström one [which is indicated as Method (b)]. The empty areas indicate that the error is greater than 1 (or overflow occurs).

Step size h	Method (a)	Method (b)
$\frac{16}{125}$		1.0×10^{-1}
$\frac{8}{125}$		6.3×10^{-3}
$\frac{4}{125}$		3.9×10^{-4}
$\frac{2}{125}$	3.1×10^{-1}	2.5×10^{-5}
$\frac{1}{125}$	4.2×10^{-2}	1.6×10^{-6}
$\frac{1}{250}$	8.0×10^{-3}	9.9×10^{-8}
$\frac{1}{500}$	4.0×10^{-3}	4.8×10^{-9}
$\frac{1}{1000}$	2.0×10^{-3}	2.4×10^{-10}

For this problem $v = \sqrt{1/r}$, where $r = \sqrt{(y^2 + z^2)^3}$. In Table IV we present the absolute maximum error. We note here that we have obtained similar results with the change of the initial conditions of the problem.

From the above results it can be seen that the present method is much more accurate than the classical one.

VI. CONCLUSIONS

An approach for constructing efficient symplectic Runge-Kutta-Nyström methods is introduced in this paper. The present approach is based on the combination of the well-known exponential fitting technique and the symplecticness conditions. Using this approach we can construct exponentially and trigonometrically fitted symplectic Runge-Kutta-Nyström methods. Based on this approach, a very simple one-stage exponentially and trigonometrically fitted symplectic Runge-Kutta-Nyström method is developed for the numerical solution of Hamiltonian problems. Numerical examples indicate that the present method is more efficient than the classical one. We note that the proposed method has similar efficiency in systems of coupled oscillators with different frequencies. We also note that the role of symplecticity is very crucial since the symplectic exponentially fitted methods give much better results in large intervals of integration than the symplectic methods and the classical methods, i.e., methods without the symplecticness conditions.

All computations were carried out using double precision arithmetic (16 significant digits accuracy).

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