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Exponentially Fitted Symplectic Runge-Kutta-Nyström methods

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Abstract: In this work we consider symplectic Runge Kutta Nyström (SRKN) methods with three stages. We construct a fourth order SRKN with constant coefficients and a trigonometrically fitted SRKN method. We apply the new methods on the two-dimentional harmonic oscillator, the Stiefel-Bettis problem and on the computation of the eigenvalues of the Schrödinger equation.

Keywords: Runge Kutta Nyström methods, symplectic methods, exponential fitting

1. Introduction

Hamiltonian systems are systems of first order ordinary differential equations that can be expressed as

$$p' = -\frac{\partial H}{\partial q}(p,q,x), \quad q' = \frac{\partial H}{\partial p}(p,q,x), \tag{1}$$

where $(p,q) \in U$ an open subset of $\Re^{2d}$, $x \in I$ an open subinterval of $\Re$, the integer d is the number of degrees of freedom. The hamiltonian function $H(p,q,x)$ is a twice continously differentiable function on $U \times I$ that represents the total mechanical energy. The q variables are generalized coordinates and the p variables are the conjugated generalized momenta. The solution operator of a Hamiltonian system is a symplectic transformation.

A symplectic numerical method preserves the symplectic structure in the phase space when applied to Hamiltonian problems. Therefore symplectic numerical methods have been used for the numerical integration of hamiltonian problems over the past two decades. In this work we shall consider problems with separable Hamiltonian of the special form

$$H(p,q,x) = \frac{1}{2}p^T p + V(q,x), \tag{2}$$

then the Hamiltonian system has the form

$$p' = -\frac{\partial}{\partial q}V(q,x), \quad q' = p. \tag{3}$$

or

$$q'' = -\frac{\partial}{\partial q}V(q,x). \tag{4}$$

The last is a system of second order differential equations and have been treated in the literature by Runge-Kutta-Nyström (RKN) and symplectic RKN (SRKN) methods. The theory of these methods can be found in the book of Sanz-Serna and Calvo [4].

On the other hand the solution of hamiltonian systems often has an oscillatory or periodic behavior and special methods that take into acount these properties of the solution have been considered. Among these methods are frequency dependent methods as exponentially, trigonometrically fitted, phase fitted and amplification fitted methods and methods with constant coeficients as minimum phase lag, minimum amplification error, P-stable methods. Exponentially fitted methods integrate exactly differential systems whose solutions can be expressed as linear combinations of functions of the form $\exp(\lambda x), \exp(-\lambda x)$ or $\sin(\lambda x)$, $\cos(-\lambda x)$. A detailed survey of these methods can be found in Ixaru and Vanden Berghe. Simos [5] first constructed an exponentially fitted Runge-Kutta method

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that integrates exactly the test equation $y'' = -w^2 y$. More recently some authors [2] [3] have proposed several exponentially fitted RKN methods. The idea of combining symplecticity with exponential fitting was first introduced by Simos and Aguiar [6] for RKN methods, they presented a two stages modified second order symplectic RKN, also Vyver [7] constructed a two stages modified second order symplectic RKN method that integrates exactly the exponential function at the internal stage also.

Van de Vyver [8] first constructed a symplectic Runge-Kutta-Nyström method with minimum phase-lag. His method has third algebraic order and sixth phase-lag order.

In this work we present two three stages symplectic RKN methods, one with constant coefficients and fourth algebraic order and symplectic modified RKN method which integrates exactly the test equation $y'' = -w^2 y$ following the approach of Simos. In section two the basic theory of SRKN methods and exponential fitting is presented, the new methods are developed in section 3. Numerical results and conclusions are presented in section 4.

2. Symplectic RKN methods

We consider systems of second order ODEs of the form

$$y''(x) = f(x, y(x)), \quad x \in [x_0, X],$$

with initial conditions

$$y(x_0) = y_0, \quad y'(x_0) = y'_0.$$

An explicit RKN method is of the form

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{i=1}^{s} \beta_i f_i,$$

$$y'_{n+1} = y'_n + h \sum_{i=1}^{s} b_i f_i, \tag{5}$$

where

$$f_i = f\left(x_n + c_i h\, ,\, y_n + c_i h y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} f_j \right)$$

and is associated with the Butcher tableau

$$\begin{array}{c|cccc} c_1 & & & & \\ c_2 & a_{21} & & & \\ c_3 & a_{31} & a_{32} & & \\ \vdots & \vdots & \vdots & & \\ c_s & a_{s1} & a_{s2} & \cdots\, a_{s,s-1} & \\ \hline & \beta_1 & \beta_2 & \cdots\, \beta_{s-1} & \beta_s \\ \hline & b_1 & b_2 & \cdots\, b_{s-1} & b_s \end{array}$$

Suris showed that a RKN method is symplectic when applied to Hamiltonian problems of the form (2) if the coefficients of the method satisfy

$$\beta_i = b_i(1 - c_i), \qquad 1 \le i \le s, \tag{6}$$

$$b_i(\beta_j - \alpha_{ij}) = b_j(\beta_i - \alpha_{ji}), \qquad 1 \le i, j \le s. \tag{7}$$

A RKN method that satisfies (6) and (7) is called symplectic RKN method (SRKN). In the case of explicit RKN methods the coefficients a_{ij} are fully determined by the coefficients b_i and c_i

$$a_{ij} = b_j(c_i - c_j). \tag{8}$$

Condition (6) is a well known simplifying assumption from the standard theory of RKN methods that reduces the number of order conditions. Calvo and Sanz-Serna has shown that condition (7) is also a simplifying assumption. The order conditions up to fourth order method are

first order

$$b.e = 1,$$

second order

$$b.c.e = \frac{1}{2},$$

third order

$$b.c^2.e = \frac{1}{3}, \quad b.a.e = \frac{1}{6},$$

fourth order

$$b.c^3.e = \frac{1}{4}, \quad b.a.c.e = \frac{1}{24}.$$

3. Construction of the new methods

We consider the three stage method

$$\begin{array}{c|ccc} c_1 & & & \\ c_2 & b_1(c_2 - c_1) & & \\ c_3 & b_1(c_3 - c_1) & b_2(c_3 - c_2) & \\ \hline & b_1(1 - c_1) & b_2(1 - c_2) & b_3(1 - c_3) \\ \hline & b_1 & b_2 & b_3 \end{array}$$

In order to construct the fourth order method we solve the six conditions and derive the following coefficients

$$b_1 = \frac{3 - 2\sqrt{3}}{12}, \quad b_2 = \frac{1}{2}, \quad b_3 = \frac{3 + 2\sqrt{3}}{12},$$
$$c_1 = \frac{3 + \sqrt{3}}{6}, \quad c_2 = \frac{3 - \sqrt{3}}{6}, \quad c_3 = c_1.$$

Here we construct new trigonometrically fitted RKN method following the approach introduced by Simos [5] for Runge-Kutta methods. These methods integrate exactly the test equation

$$y'' = -w^2 y$$

For the exponentially fitted case we want the numerical method to integrate exactly the exponential function $\exp(\pm wx)$ with w real

$$\exp(\pm v) = 1 \pm v + (\beta.e)v^2 \pm (\beta.C.e)v^3 + (\beta.A.e)v^4$$
$$\pm(\beta.A.C.e)v^5 + (\beta.A.A.e)v^6,$$

$$\exp(\pm v) = 1 \pm (b.e)v + (b.C.e)v^2 \pm i(b.A.e)v^3$$
$$+(b.A.C.e)v^4 \pm (b.A.A.e)v^5,$$

where $v = w\,h$. For the trigonometrically fitted case we want the numerical method to integrate the exponential function $\exp(iwx)$ with w real

$$\exp(iv) = 1 + iv - (\beta.e)v^2 - i(\beta.C.e)v^3 + (\beta.A.e)v^4 + i(\beta.A.C.e)v^5 - (\beta.A.A.e)v^6,$$

$$\exp(iv) = 1 + i(b.e)v - (b.C.e)v^2 - i(b.A.e)v^3 + (b.A.C.e)v^4 + i(b.A.A.e)v^5,$$

or equivalently

$$\begin{aligned} \cos v - 1 &= -(\beta.e)v^2 + (\beta.A.e)v^4 - (\beta.A.A.e)v^6, \\ \frac{\sin v}{v} &= 1 - (\beta.C.e)v^2 + (\beta.A.C.e)v^4, \\ \cos v - 1 &= -(b.C.e)v^2 + (b.A.C.e)v^4, \qquad (9) \\ \frac{\sin v}{v} &= (b.e) - (b.A.e)v^2 + (b.A.A.e)v^4, \end{aligned}$$

We let $c_1 = 0$ from the trigonometrical fitting conditions (9) we obtain the coefficients

$$c_3 = \frac{c_2 v + (-1 + c_2(-1 + b_1 v^2))(v\cos v - \sin v)}{v(1 + (-1 + b_1 c_2 v^2)\cos v - c_2 v \sin v)}$$

$$b_3 = -\frac{(1 + (-1 + b_1 c_2 v^2)\cos v - c_2 v \sin v)^2}{p}$$

$$b_2 = \frac{-2 + (2 - b_1 v^2)\cos v + (1 + b_1)v\sin v}{p}$$

$$p = v(v + b_1(-1 + c_2)c_2 v^3)v\cos v + (-1 + (1 + b_1)c_2 v^2 - c_2^2 v^2)v \sin v$$

We have two free parameters c_2 and b_1 and we use them in order to obtain the higher possible algebraic order when $v = 0$. This is the case for

$$c_2 = \frac{1}{3} - \frac{1}{6}\sqrt{1+k} - 1/6\sqrt{2 - k + \frac{2}{\sqrt{1+k}}},$$

$$k = -\frac{3^{2/3}}{2(-3 + 2\sqrt{3})^{1/3}} + \frac{3^{1/3}(-3 + 2\sqrt{3})^{1/3}}{2}$$

$$b_1 = \frac{-3c_2 + 24c_2^2 - \sqrt{3}\sqrt{-8c_2 + 39c_2^2 - 72c_3^3 + 48c_4^4}}{12(2c_2 + 3c_2^2)}$$

(or $c_2 = -0.18799161879915978201$ and $b_1 = 0.552924973878536667$).
The classical method (for $v = 0$) has algebraic order 3 and the first condition of the fourth order is also satisfied.

For small values of h we use the following Taylor expansions

$$\begin{aligned} b_2 = &-0.18799161879915978201 + 0.01482303183011970544 7\,v^2 \\ &-0.00065676356989888196 74\,v^4 + 0.0000500899926190375665 9\,v^6 \\ &-2.2837596032644413\,10^{-6}\,v^8 + 1.6950437269127458\,10^{-7}\,v^{10}, \end{aligned}$$

$$\begin{aligned} b_3 = &\ 0.635066644920623115 - 0.0148230318301197054 5\,v^2 \\ &-0.0014383992816085817 91\,v^4 + 0.0000827946627077300777\,v^6 \\ &-1.4655145815655087\,10^{-6}\,v^8 + 2.9118114430067654\,10^{-8}\,v^{10}, \end{aligned}$$

$$\begin{aligned} c_3 = &\ 0.73166990421824007504 - 0.011642558630267127 75\,v^2 \\ &-0.00035477279557280887 4\,v^4 - 0.0000250077938624870232\,v^6 \\ &-5.568816130391094\,10^{-7}\,v^8 - 5.801982609741059\,10^{-8}\,v^{10}. \end{aligned}$$

4. Numerical Results

We shall compare our new methods Meth1 (constant coefficients) and Meth2 (variable coefficients) with the third algebraic order with 6th phase lag order SRKN method of Vyver [8] and the fourth order five stages SRKN method of Calvo and Sanz-Serna.

4.1. The two-dimentional harmonic oscillator

We consider the two-dimentional harmonic oscillator

$$p_1' = -w_1\, q_1, \quad q_1' = p_1 \quad p_2' = -w_2\, q_2, \quad q_2' = p_2$$

with initial conditions

$$p_1(0) = 0, \quad q_1(0) = 1, \quad p_2(0) = 1, \quad q_2(0) = 0.$$

The Hamiltonian of this problem is

$$H(p_1, p_2, q_1, q_2) = T(p_1, p_2) + V(q_1, q_2),$$

$$T(p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2),$$

and

$$V(q_1, q_2) = -\frac{1}{2}(w_1\, q_1^2 + w_2\, q_2^2).$$

The exact solution is

$$q_1(x) = \cos w_1\, x, \quad q_2(x) = \sin w_2\, x,$$

we choose $w_1 = w_2 = 1$. For this choise we use $v = h$. In Table 1 we present he norm of the error in the solution (first line) and the error in the Hamiltonian (second line) for the two-dimestional harmonic oscillator with integration interval $[0, 1000]$ and several stepsizes.

h	$Meth1$	$Meth2$	$Vyver3$	$CSS4$
1	$4.41\,10^{-1}$	$4.39\,10^{-6}$	$3.14\,10^{-2}$	$7.52\,10^{-2}$
	$7.11\,10^{-5}$	$6.66\,10^{-15}$	$3.01\,10^{-5}$	$3.50\,10^{-7}$
1/2	$2.32\,10^{-2}$	$9.52\,10^{-10}$	$5.36\,10^{-4}$	$4.61\,10^{-3}$
	$2.26\,10^{-7}$	$1.65\,10^{-15}$	$9.63\,10^{-8}$	$9.87\,10^{-10}$
1/4	$1.42\,10^{-3}$	$2.39\,10^{-13}$	$1.60\,10^{-5}$	$2.89\,10^{-4}$
	$8.41\,10^{-10}$	$4.77\,10^{-15}$	$3.59\,10^{-10}$	$3.57\,10^{-12}$

Table 1: *The norm of the error in the solution and the error in the Hamiltonian for the two-dimentional harmonic oscillator.*

4.2. An orbit problem studied by Stiefel and Bettis

We consider the following almost periodic orbit problem studied by Stiefel and Bettis

$$p_1' = -q_1 + 0.001\cos(x), \quad q_1' = p_1,$$
$$p_2' = -q_2 + 0.001\sin(x), \quad q_2' = p_2$$

with initial conditions

$$p_1(0) = 0. \quad q_1(0) = 1, \quad p_2(0) = 0.9995, \quad q_2(0) = 0.$$

The analytical solution is given by

$$q(x) = \cos(x) + 0.0005x\sin(x),$$
$$p(x) = \sin(x) - 0.0005x\cos(x).$$

In Table 2 we present he norm of the error in the solution for this problem with integration interval $[0, 1000]$ and several stepsizes.

h	$Meth1$	$Meth2$	$Vyver3$	$CSS4$
$1/2$	$2.38\,10^{-2}$	$3.68\,10^{-5}$	$4.66\,10^{-4}$	$4.78\,10^{-3}$
$1/4$	$1.42\,10^{-3}$	$2.22\,10^{-6}$	$1.33\,10^{-5}$	$2.98\,10^{-4}$
$1/8$	$8.78\,10^{-5}$	$1.38\,10^{-7}$	$1.74\,10^{-6}$	$1.86\,10^{-5}$
$1/16$	$5.48\,10^{-6}$	$8.58\,10^{-9}$	$2.19\,10^{-7}$	$1.16\,10^{-6}$

Table 2: *The norm of the error in the solution for the Stiefel-Bettis problem.*

4.3. Computation of the eigenvalues of the Schrödinger equation

We shall use our new methods for the computation of the eigenvalues of the one-dimensional time-independent Schrödinger equation. The Schrödinger equation may be written in the form

$$-\frac{1}{2}\psi'' + V(x)\psi = E\psi$$

where E is the energy eigenvalue, $V(x)$ the potential, and $y(x)$ the wave function.

4.3.1. The harmonic oscillator

We consider the harmonic oscillator potential

$$V(x) = \frac{1}{2}kx^2$$

with boundary conditions $\psi(-R) = \psi(R) = 0$.
We consider $k = 1$.
The exact eigenvalues are given by

$$E_n = n + \frac{1}{2}, \quad n = 0, 1, 2, \ldots$$

	R	Meth1	Meth2	Vyver3	CSS
E_0	5	0	0	0	0
E_{10}	7	7	0	0	2
E_{30}	10	160	3	2	32
E_{50}	12	739	4	12	149
E_{100}	16	6123	9	187	1179
E_{150}	19	–	13	971	3977
E_{200}	22	–	18	3171	–
E_{300}	26	–	35	–	–
E_{400}	30	–	92	–	–

Table 3: *Absolute Error* ($\times 10^{-6}$) *of the eigenvalues of the harmonic oscillator* ($h = 0.05$).

4.3.2. The doubly anharmonic oscillator

The potential of the doubly anharmonic oscillator is

$$V(x) = \frac{1}{2}x^2 + \lambda_1 x^4 + \lambda_2 x^6$$

we take $\lambda_1 = \lambda_2 = 1/2$ The integration interval is $[-R, R]$. In Table 4 we give the computed eigenvalues up to E_{20} with step $h = 1/40$ and $R = 3$.

	Meth1	Meth2	Vyver3	CSS
54.222484	117	17	3	20
67.29805	220	25	5	40
81.262879	384	35	9	71
96.061534	630	49	13	120
111.647831	987	64	19	190
127.982510	1486	81	28	288
145.031661	2162	102	38	424
162.765612	3067	123	60	613
181.158105	–	137	85	829
200.185694	–	147	121	1123

Table 4: *Absolute Error* ($\times 10^{-6}$) *of the eigenvalues of the doubly anharmonic oscillator* ($h = 1/40$).

We see that the performance of the trigonometrically fitted method is superior in comparison to the other methods tested. Furthemore the computational cost is the same for the three methods with three stages only the 4th order method of Calvo and Sanz-Serma is more expensive.

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