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Diagonally Implicit Symplectic Runge-Kutta Methods with Special Properties

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Abstract: The numerical integration of Hamiltonian systems is considered in this paper. Diagonally implicit Symplectic Runge-Kutta methods with special properties are presented. The methods developed have six and seven stages algebraic order up to 5th and dispersion order up to 8th.

Keywords: Runge Kutta methods, symplectic methods, Diagonally implicit, Phase-lag

1 Introduction

The numerical integration of Hamiltonian systems by symplectic methods has been considered by many authors. Let U be an open subset of $\Re^{2d}$, I an open subinterval of $\Re$ then the hamiltonian system of differential equations is given by

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

where $(p,q) \in U$, $x \in I$, the integer d is the number of degrees of freedom and $H(p,q,x)$ be a twice continously differentiable function on $U \times I$. The q variables are generalized coordinates, the p variables are the conjugated generalized momenta and $H(p,q)$ is the total mechanical energy. The solution operator of a Hamiltonian system is a symplectic transformation. Since symplecticity is a characteristic property of Hamiltonian systems, it is natural to search for numerical methods that share this property. The theory of these methods can be found in the books of Hairer, Lubich, Wanner [1] and Sanz Serna, Calvo [2].

The first work on symplectic numerical methods is due to de Vogelaere (1956) [3] and Ruth (1983) [4]. Ruth [4] constructed a symplectic Partitioned Runge-Kutta (PRK) method of third algebraic order. Work on symplectic Runge-Kutta methods started around 1988 when order conditions for symplecticity were derived independently by Suris [5], Lasagni [6] and Sanz-Serna [7].

Additionally the solution of Hamiltonian systems often has an oscillatory behavior and have been solved in the literature with methods which take into account the nature of the problem (see [8-14]).

There are two categories of such methods with coefficients depending on the problem and with constant coefficients. For the first category a good estimate of the period or of the dominant frequency is needed, such methods are exponetially and trigonometrically fitted methods, phase-fitted and amplification fitted methods (see [15-27]). In the second category are methods with minimum phase-lag and P-stable methods and are suitable for every oscillatory problem (see [28-29]).

The idea of combining symplecticity with exponential fitting was first introduced by Simos and Aguiar [30] for RKN methods. Since then a lot of work has been done in the construction of symplectic RK, PRK and RKN methods that are also exponetially fitted or trigonometrically fitted (see [31-34]). Van de Vyver [35] constructed a symplectic RKN method with minimum phase-lag. The authors -constructed symplectic PRK methods with minimum phase-lag (Monovasilis et. al. [36], Monovasilis [37]).

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It is well known that symplectic Runge-Kutta methods cannot be explicit. Sanz-Serna and Abia (1991) [38] constructed a fourth order symmetric and symplectic Diagonally Implicit RK (DIRK) method with three stages. Here we construct symplectic DIRK methods of algebraic orders 4 and 5 and phase-lag orders up to 8.

The theory of symplectic RK methods is given in section 2, phase-lag analysis of RK methods is given in section 3 and the new methods are constructed in section 4. Numerical results are given for the harmonic oscillator, the cubic oscillator, the pendulum problem and the two-body problem (section 5).

2 Symplectic Runge-Kutta methods

The RK method is symplectic when the coefficients of the method satisfy the relations (see Sanz-Serna [2])

$$b_i a_{ij} - b_j a_{ji} - b_i b_j = 0. \qquad (1)$$

The above relations imply that symplectic RK methods cannot be explicit. Under the assumption that $b_i \neq 0$ there exist symplectic diagonally implicit RK methods. In that case the coefficients b_i fully determine the method, since the coefficients a_{ij} can be written as

$$a_{ij} = b_j \quad \text{for} \quad i \neq j, \qquad a_{ij} = b_i/2 \quad \text{for} \quad i = j.$$

For the diagonally implicit symplectic method each stage can be expressed in terms of the previous stage

$$\begin{aligned} Y_1 &= y_n + b_1 h f_1, \\ Y_{i+1} &= Y_i + \frac{h}{2}(b_i f_i + b_{i+1} f_{i+1}) \\ y_{n+1} &= Y_s + \frac{h}{2} b_s f_s \end{aligned}$$

where $f_i = f(x_n + c_i h, Y_i)$. For each stage a non linear system of equations needs to be solved while for implicit method for each step a non linear system of equations. The symplecticness requirments act as simplifying assumptions on the order conditions and the number of order conditions needed for each order are reduced significantly.

Number of order conditios

Order	RK	SRK
1	1	1
2	2	1
3	4	2
4	8	3
5	17	6
6	37	10

The order conditions up to order 5 are

$$\text{(1st)} \sum_{i=1}^{s} b_i = 1,$$

$$\text{(3rd)} \sum_{i=1}^{s} b_i c_i^2 = 1/3,$$

$$\text{(4rd)} \sum_{i=1}^{s} b_i c_i^3 = 1/4,$$

$$\text{(5th)} \sum_{i=1}^{s} b_i c_i^4 = 1/5,$$

$$\sum_{i=1}^{s} b_i c_i^2 a_{ij} c_j = 1/10,$$

$$\sum_{i=1}^{s} b_i c_i a_{ij} a_{jk} a_{kl} c_l = 1/5!.$$

Another helpfull result is that if a method is symmetric and has even order p then the algebraic order conditions of the $p+1$ order are also satisfied.

3 Phase-lag analysis of Runge-Kutta methods

The phase-lag (or dispersion) property was introduced by Brusa and Nigro (1980) [39] and was extended to RK(N) methods by Van der Houwen and Sommeijer in their works [40], [41]. Based on the reasons fully described in Van der Houwen and Sommeijer [40] we shall confine our considerations to homogeneous phase-lag. Let ω a real number and the test equation $y' = i\omega y$ with analytical solution $y(x) = y_0 \exp(i\omega x)$. Application of the Runge Kutta method to the test equation produces the numerical solution

$$y_{n+1} = R(iv) y_n \qquad R(v) = 1 + vb(I - vA)^{-1} e$$

where $v = \omega h$.

The phase lag order of a RK method is defined as the order of approximation of the argument of the exponential function by the argument of P along the imaginary axis $\phi(v) = v - arg(R(iv))$. Then the method is said to be dispersive of order q if

$$\phi(v) = O(v^{q+1}).$$

We collect the real and imaginary parts $R(iv) = A(v^2) + ivB(v^2)$ then the dispersion can be written as

$$\phi(v) = v - \arctan\left(v \frac{B(v^2)}{A(v^2)} \right).$$

We consider Taylor expansion of the stability function $R(z)$

$$R(z) = \beta_0 + \beta_1 z + \beta_2 z^2 + \cdots + \beta_n z^n + \cdots.$$

The following result is due to Franco et. al. [42] although an equivalent form is given by Van Der Houwen and Sommeijer in [40].

A RK method is dispersive of order q if the coefficients β_j in the Taylor expansion of $R(z)$ satisfy the following conditions:

$$\frac{\beta_0}{j!} - \frac{\beta_1}{(j-1)!} + \frac{\beta_2}{(j-2)!} - \cdots + (-1)^j \beta_j = 0, \quad j = 1,3,\ldots,q-1,$$

and in addition q is even.

A method of algebraic order p has at least dispersion order $p+1$ if p odd and p if p even.

4 Construction of the new methods

We shall consider methods with six and seven stages. The stability function for the s stage diagonally implicit symplectic method is

$$R(v) = \frac{\prod_{i=1}^{s}(2+b_i v)}{\prod_{i=1}^{s}(-2+b_i v)}$$

Since the method is symmetric only the two conditions for algebraic order 3 are needed to ensure fourth algebraic order we also solve the phase-lag conditions of order 6 which becomes $\beta_5 = 1/5!$. We obtain the following coefficients (*Meth546, the first number denotes the number of stages, the second the algebraic order and the third the dispersion order of the method*):

$$b_1 = -2.150611289942181,$$
$$b_2 = 1.452223059167718,$$
$$b_3 = 2.3967764615489258.$$

Here we constructed a six stages method with algebraic order 5 since there are 6 order conditions for algebraic order 5. This method also has phase-lag order 6 (*Meth656*). The coefficients of the method are:

$$b_1 = 0.5080048194000274,$$
$$b_2 = 1.360107162294827,$$
$$b_3 = 2.0192933591817224,$$
$$b_4 = 0.5685658926458251,$$
$$b_5 = -1.4598520495864393,$$
$$b_6 = -1.9961191839359627.$$

We have constructed a fifth order method with seven stages with the assumption $b_7 = b_1$ and imposing the six order conditions of order 5 (*Meth756*)

$$b_1 = -1.9119528632302611$$
$$b_2 = 1.7330487520694027$$
$$b_3 = 1.7978839093830516$$
$$b_4 = 1.2522794817510428$$
$$b_5 = 2.87965671639611$$
$$b_6 = -2.8389631331390848.$$

We also construct a symmetric method with seven stages, we have four coefficients to determine (b_1,b_2,$b_3$and b_4). We impose the two conditions of order three then the method has algebraic order four. The conditions for dispersin order 6 and 8 are

$$\beta_5 = \frac{1}{5!}, \quad \beta_6 - \beta_7 = \frac{6}{7!}$$

we also impose these conditions. The coefficients of this method (*Meth748*) are:

$$b_1 = 1.4944291445422252$$
$$b_2 = -2.3484252147655893$$
$$b_3 = 2.8982950506987870$$
$$b_4 = 1 - 2b_1 - 2b_2 - 2b_3.$$

5 Numerical Results

The new methods as well as the fourth order method of Sanz Serna and Abia [38] (*Meth344*) are tested for the harmonic oscillator, the cubic oscillator, the pendulum problem and the two-body problem. The hamiltonian for all problems considered is separable with quadratic kinetic energy

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

This leads to a favourable implementation in terms of the non linear system. For the one dimensional problems (harmonic, cubic oscillator and pendulum) only a non linear equation needs to be solved at each stage while for the two body problem a system of two non linear equations needs to be solved at each stage.

5.1 Harmonic Oscillator

The Hamiltonian of this problem is

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

and the equations of motion are

$$p' = -q, \quad q' = p.$$

We consider the initial conditions $p(0) = 1$, $q(0) = 0$, then the exact solution is $p(x) = \cos x$, $q(x) = \sin x$.

The problem has been solved numerically in the interval $[0, 10^3]$ with several steps. In Table 1 we present the maximum absolute error of the solution. The error of the Hamiltonian for all methods is less than 10^{-15}.

Table 1: *Maximum absolute error of the solution of the Harmonic Oscillator.*

h	*Meth344*	*Meth546*	*Meth656*	*Meth748*	*Meth756*
0.5	−−	−−	$1.26\,10^{-1}$	$5.51\,10^{-1}$	$1.06\,10^{-2}$
0.2	$1.02\,10^{-1}$	$7.30\,10^{-3}$	$6.90\,10^{-4}$	$8.91\,10^{-4}$	$4.84\,10^{-5}$
0.1	$6.56\,10^{-3}$	$1.22\,10^{-4}$	$1.13\,10^{-5}$	$4.05\,10^{-6}$	$7.70\,10^{-7}$

5.2 Cubic Oscillator

The Hamiltonian of this problem is

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

and the equations of motion are

$$p' = -q + \varepsilon q^3, \quad q' = p.$$

We consider the initial conditions $p(0) = 0$, $q(0) = 1$.

The problem has been solved numerically in the interval $[0,10^3]$ for $\varepsilon = 0.01$ and $\varepsilon = 0.1$ with several steps. In tables 2 and 3 (upper part $\varepsilon = 0.01$, lower part $\varepsilon = 0.1$)we present the maximum absolute error of the Hamiltonian and the solution (all methods tested gave error greater than 1 for $h = 1$).

Table 2: *Maximum absolute error of the Hamiltonian of the Cubic Oscillator for* $\varepsilon = 0.01,\ 0.1$.

h	*Meth344*	*Meth546*	*Meth656*	*Meth748*	*Meth756*
1	$4.62\,10^{-4}$	$4.45\,10^{-4}$	$1.39\,10^{-3}$	$4.36\,10^{-4}$	$3.92\,10^{-5}$
0.5	$2.17\,10^{-6}$	$2.75\,10^{-7}$	$3.69\,10^{-6}$	$3.89\,10^{-8}$	$9.32\,10^{-8}$
0.1	$1.42\,10^{-7}$	$3.75\,10^{-9}$	$1.06\,10^{-7}$	$1.15\,10^{-9}$	$1.11\,10^{-8}$
1	$4.48\,10^{-3}$	$4.33\,10^{-3}$	$1.07\,10^{-2}$	$4.26\,10^{-3}$	$3.14\,10^{-4}$
0.5	$1.89\,10^{-5}$	$2.10\,10^{-6}$	$3.18\,10^{-5}$	$2.33\,10^{-7}$	$8.49\,10^{-7}$
0.1	$1.23\,10^{-6}$	$2.64\,10^{-8}$	$8.96\,10^{-7}$	$1.13\,10^{-8}$	$1.02\,10^{-7}$

Table 3: *Maximum absolute error of the solution of the Cubic Oscillator for* $\varepsilon = 0.01,\ 0.1$.

h	*Meth344*	*Meth546*	*Meth656*	*Meth748*	*Meth756*
0.5	$9.64\,10^{-2}$	$6.56\,10^{-3}$	$6.35\,10^{-4}$	$7.61\,10^{-4}$	$4.33\,10^{-5}$
0.1	$6.19\,10^{-3}$	$1.10\,10^{-4}$	$1.04\,10^{-5}$	$3.43\,10^{-6}$	$6.60\,10^{-7}$
0.5	$5.39\,10^{-2}$	$2.05\,10^{-3}$	$1.71\,10^{-3}$	$2.36\,10^{-4}$	$2.05\,10^{-4}$
0.1	$3.60\,10^{-3}$	$2.27\,10^{-4}$	$2.29\,10^{-4}$	$1.98\,10^{-4}$	$1.97\,10^{-4}$

5.3 Standard Pendulum

The Hamiltonian of this problem is given by

$$H(p,q) = \frac{p^2}{2} - a\cos(q), \quad a > 0.$$

The equations of motion are

$$p' = -a\sin(q), \quad q' = p.$$

We consider the problem with initial conditions

$$p(0) = 1, \quad q(0) = 0.$$

In tables 4, 5 we give the maximum absolute error of the solution and the Hamiltonian for this problem for $a = 1$ with several steps; the integration interval is $[0,10^3]$.

Table 4: *Maximum absolute error of the solution of the Pendulum.*

h	*Meth344*	*Meth546*	*Meth656*	*Meth748*	*Meth756*
0.2	$7.32\,10^{-3}$	$1.11\,10^{-4}$	$1.62\,10^{-3}$	$2.68\,10^{-5}$	$2.21\,10^{-5}$
0.1	$4.71\,10^{-4}$	$1.21\,10^{-6}$	$3.92\,10^{-5}$	$9.98\,10^{-7}$	$1.53\,10^{-6}$
0.01	$4.71\,10^{-8}$	$3.23\,10^{-10}$	$5.66\,10^{-10}$	$2.14\,10^{-10}$	$1.06\,10^{-9}$

Table 5: *Maximum absolute error of the Hamiltonian of the Pendulum.*

h	*Meth344*	*Meth546*	*Meth656*	*Meth748*	*Meth756*
0.2	$3.10\,10^{-5}$	$2.99\,10^{-6}$	$6.59\,10^{-5}$	$1.78\,10^{-7}$	$1.94\,10^{-6}$
0.1	$2.00\,10^{-6}$	$3.27\,10^{-8}$	$1.94\,10^{-6}$	$3.43\,10^{-8}$	$2.09\,10^{-7}$
0.01	$2.03\,10^{-10}$	$1.13\,10^{-11}$	$3.33\,10^{-11}$	$6.74\,10^{-12}$	$2.11\,10^{-10}$

5.4 The two-body problem

The Hamiltonian of this problem is

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

The equations of motion are

$$p_1' = -\frac{q_1}{\sqrt{(q_1^2+q_2^2)^3}}, \quad q_1' = p_1$$

$$p_2' = -\frac{q_2}{\sqrt{(q_1^2+q_2^2)^3}}, \quad q_2' = p_2.$$

with initial conditions

$$p_1(0) = 0, \qquad q_1(0) = 1-e,$$
$$p_2(0) = \sqrt{\tfrac{1+e}{1-e}}, \qquad q_2(0) = 0.$$

The exact solution is

$$q_1(x) = \cos(E) - e, \quad q_2(x) = \sqrt{1-e^2}\,\sin(E),$$

where e is the eccentricity of the orbit and the eccentricity anomaly E is expressed as an implicit function of x by Kepler's equation

$$x = E - e\sin(E).$$

In tables 6, 7 (upper part $e = 0$, middle part $e = 0.1$, lower part $e = 0.3$) we give the numerical evidence for this problem with steps $h = \pi/16$, $h = \pi/32$ the integration interval is $[0,320\pi]$.

Table 6: *Maximum absolute error of the solution of the Two-Body Problem for* $e = 0,\ 0.1,\ 0.3$.

h	*Meth344*	*Meth546*	*Meth656*	*Meth748*	*Meth756*
$\pi/16$	−−	$6.38\,10^{-1}$	$9.74\,10^{-2}$	$6.24\,10^{-1}$	$2.92\,10^{-4}$
$\pi/32$	$7.88\,10^{-2}$	$6.38\,10^{-1}$	$9.74\,10^{-2}$	$6.24\,10^{-1}$	$2.92\,10^{-4}$
$\pi/16$	−−	−−	$2.31\,10^{-1}$	−−	$3.63\,10^{-3}$
$\pi/32$	$1.15\,10^{-1}$	$1.35\,10^{-2}$	$4.05\,10^{-3}$	$2.82\,10^{-3}$	$1.88\,10^{-4}$
$\pi/16$	−−	−−	−−	−−	$8.61\,10^{-2}$
$\pi/32$	$3.84\,10^{-1}$	$1.00\,10^{-1}$	$3.33\,10^{-1}$	$5.26\,10^{-2}$	$4.85\,10^{-3}$

Table 7: *Maximum absolute error of the Hamiltonian of the Two-Body Problem for* $e = 0,\ 0.1,\ 0.3$.

h	*Meth344*	*Meth546*	*Meth656*	*Meth748*	*Meth756*
$\pi/16$	$1.09\,10^{-6}$	$2.07\,10^{-7}$	$2.41\,10^{-7}$	$2.05\,10^{-7}$	$3.01\,10^{-9}$
$\pi/32$	$3.02\,10^{-9}$	$2.37\,10^{-11}$	$3.94\,10^{-10}$	$1.19\,10^{-12}$	$4.66\,10^{-11}$
$\pi/16$	$1.64\,10^{-4}$	$8.53\,10^{-5}$	$1.24\,10^{-4}$	$1.23\,10^{-5}$	$5.70\,10^{-6}$
$\pi/32$	$8.79\,10^{-6}$	$8.62\,10^{-7}$	$4.21\,10^{-6}$	$2.17\,10^{-7}$	$6.47\,10^{-7}$
$\pi/16$	$1.52\,10^{-3}$	−−	−−	−−	$6.47\,10^{-5}$
$\pi/32$	$6.96\,10^{-5}$	$1.39\,10^{-5}$	$1.85\,10^{-4}$	$7.35\,10^{-6}$	$6.54\,10^{-6}$

5.5 Long time integration

In this section we examine the performance of methods as the integration interval increases. We shall consider the two body problem with eccentricity $e = 0$ and the pendulum problem (Figure 1, Figure 2). The methods used are the classical fourth order RK method *RK444*, *Meth344*, *Meth748*. The integration interval is $[0, 32000\pi]$ for the two body problem and $[0, 10^5]$ for the pendulum problem.

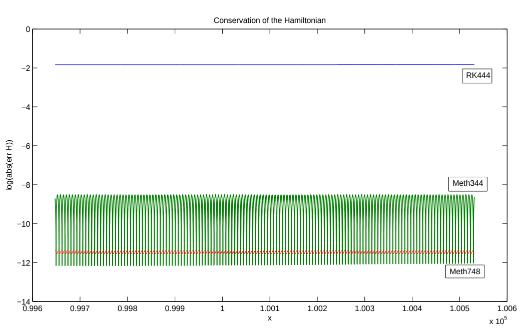

Fig. 1: Two body problem. Conservation of Hamiltonian.

6 Conclusions

Here we have constructed diagonally implicit symplectic RK methods with algebraic order up to five and dispersion order up to eight. Numerical tests have been performed on the harmonic and cubic oscillator, the pendulum and the two-body problem. In future work we shall consider symplectic DIRK methods with variable coefficients.

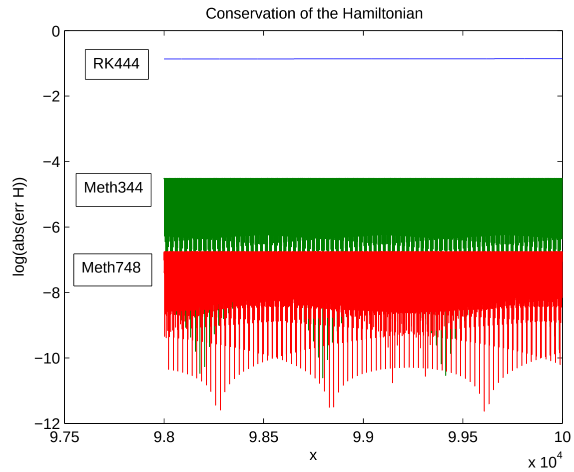

Fig. 2: Pendulum problem. Conservation of Hamiltonian.

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