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A SIXTH ORDER DIAGONALLY IMPLICIT SYMMETRIC AND SYMPLECTIC RUNGE-KUTTA METHOD FOR SOLVING HAMILTONIAN SYSTEMS*

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Abstract The paper is concerned with construction of symmetric and symplectic Runge-Kutta methods for Hamiltonian systems. Based on the symplectic and symmetrical properties, a sixth-order diagonally implicit symmetric and symplectic Runge-Kutta method with seven stages is presented, the proposed method proved to be P-stable. Numerical experiments with some Hamiltonian oscillatory problems are presented to show the proposed method is as competitive as the existing Runge-Kutta methods in scientific literature.

Keywords Oscillatory Hamiltonian system, symplecticness, symmetric, P-stable, Runge-Kutta method.

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1. Introduction

In this paper, we derive a high order symmetric and symplectic Runge-Kutta method for the numerical solution of oscillatory Hamiltonian systems. The oscillatory Hamiltonian systems often arise in different fields of applied sciences such as celestial mechanics, astrophysics, chemistry, electronics, molecular dynamics, and so on [1].

In the Hamilton formulation of classical mechanics, generalized coordinates $q_1, q_2, \cdots, q_n$ and generalized momenta $p_1, p_2, \cdots, p_n$ are used to represent the state of a mechanical system. The equations of motion are defined in terms of a Hamiltonian function $H(p_1, p_2 \cdots, p_n, q_1, q_2 \cdots, q_n)$ by the equations

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, i = 1, 2, \cdots, n, \tag{1.1}$$

where $n \geq 1$ is the number of degrees of freedom and H is the Hamiltonian function. Denote $p_i = y_i, q_i = y_{i+n}, y = (y_1, y_2, \cdots, y_{2n})^T$ and $\frac{\partial H}{\partial y} = (\frac{\partial H}{\partial y_1}, \frac{\partial H}{\partial y_2}, \cdots, \frac{\partial H}{\partial y_{2n}})^T$. Then (1.1) becomes:

$$y'(t) = J^{-1} \bigtriangledown_y H(t, y(t)), \tag{1.2}$$

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$$J = \begin{pmatrix} \boldsymbol{0} & I_n \\ -I_n & \boldsymbol{0} \end{pmatrix},\ J^{-1} = -J = J^T,$$

where I_n is an identity matrix, and $\boldsymbol{0}$ is a zero matrix.

The flow map of the Hamiltonian system (1.2) will be denoted by $\phi : \mathbf{R}^{2n} \to \mathbf{R}^{2n}$ for each fixed t_0, so that $\phi(y_0) = y(t_0 + h; t_0, y_0)$.

Definition 1.1. A numerical method defined by the flow map ϕ is called symplectic if for the Hamiltonian system (1.2), if the Jacobian matrix of $\phi_h(y_0)$ satisfies the condition

$$\phi_h'(y_0) J \phi_h'(y_0)^T = J.$$

Definition 1.2. The adjoint method ϕ_h^* of a numerical method ϕ_h is the inverse map of the original method with reversed time step $-h$, i.e., $\phi_h^* = \phi_{-h}^{-1}$. A method for which $\phi_h^* = \phi_h$ is called symmetric.

The general s-stage Runge-Kutta method is defined by:

$$\begin{aligned} Y_i &= y_n + h \sum_{j=1}^{s} a_{ij} f(x_n + c_j h, Y_j), \quad i = 1, 2, \cdots, s, \\ y_{n+1} &= y_n + h \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i). \end{aligned} \tag{1.3}$$

Lemma 1.1 ([2])**.** *Assume that the coefficients of the method (1.3) satisfy the following relationship*

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad 1 \le i, j \le s, \tag{1.4}$$

then the method is symplectic.

Lemma 1.2. *If*

$$a_{s+1-i,s+1-j} + a_{ij} = b_j, \quad \textit{for all } i,\ j, \tag{1.5}$$

then the Runge-Kutta method (1.3) is symmetric.

The design and construction of numerical methods for Hamiltonian systems has been considered by several authors [5–9, 15–20]. In [9], A. Iserles constructed symplectic Runge-Kutta methods with real eigenvalues with the help of perturbed collocation. In [19], J.M. Sanz-Serna and L. Abia gave order conditions of symplectic Runge-Kutta methods. In [7], E. Hairer and G. Wanner constructed symplectic Runge-Kutta methods using the W-transformation. In [20], G. Sun gave a simple way to symplectic methods with the help of symplectic conditions of partitioned Runge-Kutta methods. In this paper, we consider the following format Runge-Kutta methods which expressed in Butcher notation by the table of coefficients,

$$\begin{array}{c|c} \mathrm{c} & \mathrm{A} \\ \hline & b^T \end{array} = \begin{array}{c|cccc} c_1 & \frac{b_1}{2} & & & \\ c_2 & b_1 & \frac{b_2}{2} & & \\ \vdots & \vdots & \vdots & \ddots & \\ c_s & b_1 & b_2 & \cdots & \frac{b_s}{2} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}, \tag{1.6}$$

where $c_i = \sum_{j=1}^{s} a_{ij}$, and $b_i \neq 0$ $(i = 1, 2, \cdots, s)$, $a_{ij} = 0$ $(i < j)$, the methods (1.6) satisfy the condition (1.4) naturally.

The methods (1.6) have been discussed by J.M. Franco and I. Gómez [6], Z. Kalogiratou, T. Monovasilis and T.E. Simos [11,12], Qin and Zhang [15], Y.B. Suris [18] and so on. In [18], methods were derived with order $p = 3$. In [6], methods were derived with order $p = 4$. In [11], a fourth-order symmetric method with five stages was presented. In [12], a fifth-order method with six stages was presented.

In this paper, we derive a diagonally implicit symmetric and symplectic Runge-Kutta methods(DISSRK). The structure of the paper is as follows. In Section 2, using the symplectic and symmetrical properties, a sixth-order DISSRK with seven stages is presented. In section 3, the proposed method was shown to be P-stable. In section 4, numerical experiments with some Hamiltonian oscillatory problems are presented to show the proposed method is as competitive as the existing Runge-Kutta methods in scientific literature.

2. Derivation of sixth order Symmetric and symplectic Runge-Kutta methods

2.1. Order condition

Butcher [2] proves that, if the stage number s and the coefficients a_{ij}, b_i are regarded as free parameters, then each of order conditions of Runge-Kutta methods is independent of the others. However, as the format Runge-Kutta methods (1.6), which satisfy the symplectic condition (1.4) automatically, then the method coefficients are no longer free parameters and some of order conditions turn out to be superfluous, Table 1 shows the number of order conditions for general Runge-Kutta methods(RK) and symplectic Runge-Kutta methods(SRK), the number of order conditions needed for each order of SRK is reduced significantly.

Table 1. Number of order conditions for RK and SRK and DISSRK up to order 6.

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

The order conditions for symplectic Runge-Kutta methods up to order 6 are:

$$(1st)\ \sum_i b_i = 1, \quad (3rd)\ \sum_i b_i c_i^2 = 1/3, \quad (4rd)\ \sum_i b_i c_i^3 = 1/4,$$

$$(5th)\ \sum_i b_i c_i^4 = 1/5, \quad \sum_{i,j} b_i c_i^2 a_{ij} c_j = 1/10, \ \sum_{i,j,k} b_i a_{ij} c_j a_{ik} c_k = 1/20,$$

$$(6th)\ \sum_i b_i c_i^5 = 1/6, \quad \sum_{i,j} b_i c_i a_{ij} c_j^3 = 1/24, \ \sum_{i,j,k} b_i c_i a_{ij} c_j a_{jk} c_k = 1/48,$$

$$\sum_{i,j,k,l} b_i a_{ij} c_j a_{jk} a_{kl} c_l = 1/180.$$

M. Sofroniou and W. Oevel [16] proved the order conditions arising from rooted trees of even order are automatically satisfied for self-adjoint symplectic Runge-Kutta schemes. Table 1 shows the number of order conditions for DISSRK, only 5 order conditions be left over.

The order conditions for the sixth-order DISSRK are:

$$(1st)\ \sum_i b_i = 1, \quad (3rd)\ \sum_i b_i c_i^2 = \frac{1}{3},$$
$$(5th)\ \sum_i b_i c_i^4 = \frac{1}{5},\ \sum_{i,j} b_i c_i^2 a_{ij} c_j = \frac{1}{10},\ \sum_{i,j,k} b_i a_{ij} c_j a_{ik} c_k = \frac{1}{20}.$$

2.2. Derivation a sixth-order DISSRK method

It has been remarked by Hairer [8] that symmetric numerical methods show a better long time behaviour than nonsymmetric ones when applied to reversible differential equations. Our purpose is to derive a symmetrical and symplectic Runge-Kutta method with higher algebraic order and less stage order.

Let

$$\tau_1 = \sum_i b_i - 1, \quad \tau_2 = \sum_i b_i c_i^2 - \frac{1}{3}, \quad \tau_3 = \sum_i b_i c_i^4 - \frac{1}{5},$$
$$\tau_4 = \sum_{i,j} b_i c_i^2 a_{ij} c_j - \frac{1}{10}, \quad \tau_5 = \sum_{i,j,k} b_i a_{ij} c_j a_{ik} c_k - \frac{1}{20},$$
$$T = (\tau_1, \tau_2, \tau_3, \tau_4, \tau_5).$$

To derive a sixth-order diagonally implicit symmetrical and symplectic Runge-Kutta method of format (1.6) with seven stages, we only need let $b1 = b7,\ b2 = b6,\ b3 = b5$ and choose the favorable free parameters b_i $(i = 1, 2, \cdots, 4)$ to minimize the error norm $A = \|T\|_2$.

We have the best results, that is the parameters $b_i(1, 2, \cdots, 4)$ and the corresponding value A in Table 2.

Table 2. The value of $b_i (i = 1, 2, \cdots, 4)$ and A.

b_1	b_2	b_3
7.8451361047755652e-01	2.3557321335935860e-01	-1.1776799841788705e+00

b_4	A
1.3151863206839107e+00	1.450959051957807e-016

3. P-stable of DISSRK methods

In this section, we will investigate P-stable of the proposed method. Methods preserving the amplitudes of the Hamiltonian oscillatory systems for arbitrary large value λ and large step-size lengths are called P-stable (see [10]). The concept of P-stability has been considered in the literature for multistage and multi-step methods,

including Runge-Kutta methods, Nyström methods, multi-step methods and some hybrid methods(see [3, 4, 6, 10, 13, 14]).

Considering a scalar test ordinary differential equation

$$y' = \lambda y, \quad \lambda \in C \;\; Re(\lambda) < 0.$$

Applying (1.3) to the test equation yields the stability difference equation of the form

$$y_{n+1} = R(z)y_n, \;\; z = \lambda h$$

where $R(z) = 1 + zb^T(I - zA)^{-1}e$ is the stability function of the method, and I is an identity matrix, and $e = (1, 1, \cdots, 1)^T$.

Definition 3.1 ([6])**.** A Runge-Kutta method with stability function $R(z)$ is said to be P-stable if it satisfies $|R(iv)| = 1$,$\forall v \in \mathbb{R}$, $i = \sqrt{-1}$.

For symplectic Runge-Kutta methods of format (1.6), we always have

$$R(\mu) = \frac{det(I + \mu A)}{det(I - \mu A)}, \quad \mu = iv,$$

since the coefficients of the rational polynomial $R(\mu)$ are real, for symmetrical Runge-Kutta methods, we always have $|R(\mu)| = 1$. So we have the following Theorem.

Theorem 3.1. *The proposed symmetrical and symplectic Runge-Kutta method is P-stable.*

4. Numerical experiments

In this numerical study, we are interested in the errors of the Hamiltonian quantity. Four well known Hamiltonian problems from the literature were chosen for our test.

We compare the proposed method which denoted by **DISSRK76** with some already known methods, which denoted by:

1 **M756**: A fifth-order method of format (1.6) with seven stages which has dispersion order 6(see [11]), but it is not a symmetrical one.

2 **Explicit**: The explicit sixth-order Runge-Kutta method with seven stages .

3 **Lobatto**: Lobatto IIIA(s=4,p=6), a sixth-order symmetrical Runge-Kutta method with four stages, not a symplectic one.

Problem 1. Harmonic oscillatory system

The harmonic oscillatory system given below:

$$q' = p, \;\; p' = -q. \tag{4.1}$$

The Hamiltonian function is:

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

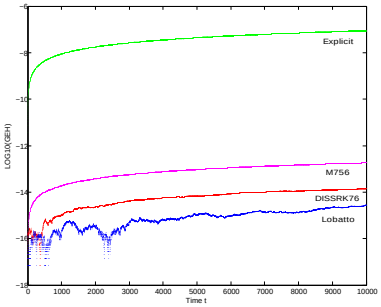

Figure 1. Errors if the Hamiltonian function of (4.1) on [0,10000]

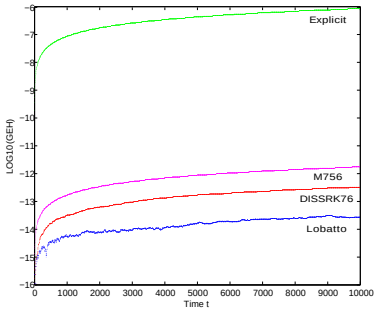

Figure 2. Errors if the Hamiltonian function of of (4.2) on [0,10000]

The exact solution is:

$$\begin{pmatrix} p(t) \\ q(t) \end{pmatrix} = \begin{pmatrix} cos(t) & -sin(t) \\ sin(t) & cos(t) \end{pmatrix} \begin{pmatrix} p(0) \\ q(0) \end{pmatrix},$$

where $p(0) = -0.1,\ q(0) = 0.3$.

Figure 1 shows the Hamiltonian quantity error $GEH = \|H_n - H_0\|$ of the compared methods on the interval $t \in [0, 10000]$, and the step-size $h = \pi/30$, $H_0 = 1/2(p^2(0) + q^2(0))$. From the figure, we can see, the accuracy of the **DISSRK76** is slightly inferior to the **Lobatto**, and more better than the **M756** and the **explicit** method. The **Lobatto** is more accuracy than the **DISSRK76**, for the reason that it has lower computational cost than the **DISSRK76** when solving problem 1.

Problem 2. Homogeneous linear system

The equations of motion are

$$p_1' = -q_1, \quad p_2' = -q_2, \quad q_1' = p_1, \quad q_2' = \lambda^2 p_2, \tag{4.2}$$

with initial conditions

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

The Hamiltonian function is:

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

which is a stiff problem with $\lambda = 10^{10}$.

Figure 2 shows the Hamiltonian quantity error $GEH = \|H_n - H_0\|$ of the compared methods on the interval $t \in [0, 10000]$, and the step-size $h = \pi/30$, $H_0 = 1/2(p_1^2(0) + \lambda^2 p_2^2(0)) - 1/2(q_1^2(0) + q_2^2(0))$. From the figure, we can see, the results is similar to the previous problem. The performance of three implicit methods is superior to the explicit method when solving the problem.

Problem 3. The Mathematical Pendulum

It is a famous model of nonlinear differential equations in classical mechanics can be written as

$$p' = -\sin q, \qquad q' = p. \tag{4.3}$$

The Hamiltonian function is:

$$H = \frac{1}{2}p^2 - \cos q.$$

The initial values are $p(0) = 0,\ q(0) = 0.5$.

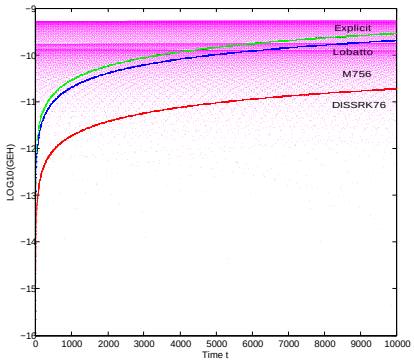

Figure 3. Errors if the Hamiltonian function of of (4.3) on [0,10000]

Figure 3 shows the Hamiltonian quantity error $GEH = \|H_n - H_0\|$ of the compared methods on the interval $t \in [0, 10000]$, and the step-size $h = \pi/120$, $H_0 = \frac{1}{2}p^2(0) - cosq(0)$. From the figure, we can see, the accuracy of the **DISSRK76** is the best one in the compared methods, the Hamiltonian error of the **M756** mainly range from 10^{-13} to 10^{-9}.

Problem 4. The two-body problem

The well-known Kepler's problem defined by

$$p_1' = -\frac{q_1}{(q_1^2 + q_2^2)^{\frac{3}{2}}},\ p_2' = -\frac{q_2}{(q_1^2 + q_2^2)^{\frac{3}{2}}},\ q_1' = p_1,\ q_2' = p_2. \tag{4.4}$$

The Hamiltonian function is

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

where $p = (p_1, p_2)^T$ and $q = (q_1, q_2)^T$ are the velocity and position vectors, with the initial conditions

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

The exact solution of this initial value problem is given by:

$$p_1(t) = -\sin(t),\quad p_2(t) = \cos(t),\quad q_1(t) = \cos(t),\quad q_2(t) = \sin(t).$$

The system has the energy $H = \frac{1}{2}(p_1^2(t) + p_2^2(t)) - \frac{1}{(q_1^2(t)+q_2^2(t))^{1/2}}$ and the angular momentum $M = q_1(t)p_2(t) - q_2(t)p_1(t)$ as conserved quantities.

Figure 4 and Figure 5 show the Hamiltonian quantity error $GEH = \|H_n - H_0\|$ and the angular momentum $GEM = \|M_n - M_0\|$ of the compared methods on the interval $t \in [0, 10000]$, and the step-size $h = \pi/120$, $h = \pi/60$ correspondingly. From the figure, we can see, the accuracy of **DISSRK76** is slightly inferior to the **Lobatto**, and more better than the **M756** and the **explicit** method.

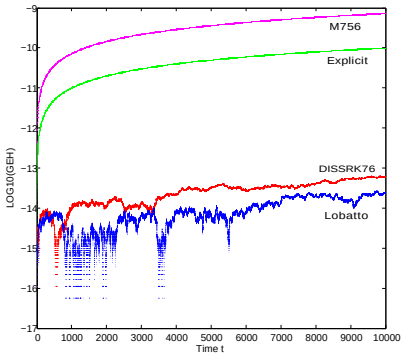

Figure 4. Errors if the Hamiltonian function of (4.4) on [0,10000]

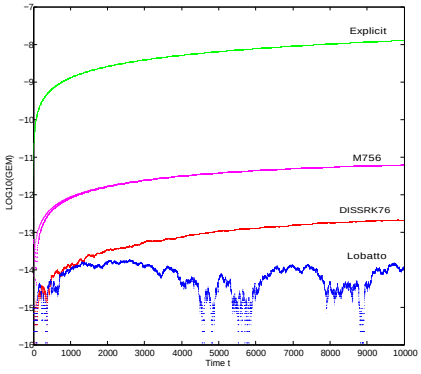

Figure 5. Errors if the Hamiltonian function of of (4.4) on [0,10000]

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