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OPTIMIZED FIFTH ORDER SYMPLECTIC INTEGRATORS FOR ORBITAL PROBLEMS

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RESUMEN

Se presenta un integrador simpléctico optimizado de quinto orden. El desarrollo de este nuevo esquema se basa en: (1) un nuevo conjunto de condiciones para los esquemas simplécticos de paso k hasta de quinto orden, y (2) el error mínimo. Los resultados numéricos muestran la eficiencia del método propuesto.

ABSTRACT

In this paper an optimized fifth algebraic order symplectic integrator is produced. The development of the new scheme is based: (1) on a new set of conditions for symplectic k-step schemes with order up to five and (2) on the minimum error. The numerical results show the efficiency of the proposed method.

Key Words: methods: data analysis — methods: miscellaneous — methods: numerical

1. INTRODUCTION

The approximate integration of Hamiltonian systems is of considerable importance to areas such as molecular dynamics, mechanics, astrophysics and others. By long-time integration of large systems it is possible to obtain better understanding of physical properties of the systems. It is well known that geometric integrators, such as symplectic and reversible integrators, are superior compared with non-symplectic methods for the integration of Hamiltonian systems (Sanz-Serna & Calvo 1994). The main characteristics of geometric integrators (which give them superiority in comparison with non-symplectic integrators) are: (1) preservation of the energy integral, (2) linear error growth and (3) correct qualitative behavior.

The Hamiltonian canonical equations are given below:

$$\begin{cases} \dot{p} = -\frac{\partial H}{\partial q} \,, \\ \dot{q} = \frac{\partial H}{\partial p} \,, \end{cases} \tag{1}$$

where the dot denotes the ordinary derivative, with q and p are the $\nu-$ dimensional vectors of the coordinates and momenta respectively and H is the Hamiltonian function:

$$H = T(p) + V(q)\,. \tag{2}$$

Several important equations have been transformed into Hamiltonian canonical equation (for example in Liu et al. 2000). Liu et al. (2000) has transformed the Schrödinger equation into Hamiltonian canonical equation using a Legendre transformation.

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During the last decade some symplectic integrators have been developed and used in mathematical packages[3]. Ruth (1983) first published symplectic methods for problems of the form (1). Integrators of order three were constructed by Ruth (1983), integrators of order four were obtained by Candy & Rozmus (1991) and Forest & Ruth (1990). Yoshida (1990) has constructed reversible symplectic integrators of sixth and eighth order. Recently Tselios & Simos (2003, 2004) have introduced optimized symplectic integrators for the numerical solution of (1).

A detailed presentation of the relevant literature can be found in Hairer, Lubich, & Wanner (2002), McLachlan (1995), McLachlan & Quispel (2006), Forest (2006), Laskar & Robutel (2001), Nadolski & Laskar (2002), Omelyan, Mryglod, & Folk (2002a,b), and Yoshida (1993).

The purpose of this paper is to introduce an optimized fifth algebraic order symplectic integrator. The production of the new scheme is based on a new set of conditions for symplectic k-step schemes with order up to five. Based on this set, forty six symplectic seven-step methods of fifth algebraic order are obtained. The optimized fifth order symplectic integrator is defined using the minimum error.

The new insights of this paper (compared with the paper of Tselios & Simos 2004) are:

- In this paper the linearly independent system of equations of the produced necessary conditions up to algebraic order five is proved.
- Based on the sixty two necessary conditions produced in order to achieve the agreement of the relations for the construction of k-step symplectic integrators of sixth algebraic order (see relations 5 and 6 below) and using the minimization of the error function, the new proposed optimized fifth algebraic order method is produced (see for more details Tselios & Simos 2011)[4].

The paper is constructed as follows. In § 2 the basic theory on symplectic integrators is presented. The construction of a new set of conditions for the fifth order k-step symplectic schemes is presented in § 3. The new proposed fifth order method is developed in § 4. Finally, in § 5 a numerical illustration of the new developed method is presented.

2. SYMPLECTIC INTEGRATORS

Our investigation on the construction of symplectic integrators is based on the procedure developed by Forest & Ruth (1990) and Liu et al. (2000):

$$\begin{cases} p_i = p_{i-1} - c_i h(\frac{\partial V}{\partial q})_{q=q_{i-1}} \\ q_i = q_{i-1} + d_i h(\frac{\partial T}{\partial p})_{p=p_i} \end{cases} \qquad i = 1, ..., k\,, \tag{3}$$

where h is a step-size and k is the number of steps. The values $(q_0,\, p_0)$, are the initial values and $(q_k,\, p_k)$ are the numerical solution at the k-step. The coefficients c_i and d_i are free parameters and the transformation from $(q_0,\, p_0)$ to $(q_k,\, p_k)$ is symplectic (Forest & Ruth 1990).

The parameters c_i and d_i are obtained by Yoshida (1990) using the relation:

$$e^{h(A+B)} = \prod_{i=1}^{k} e^{c_i hA} e^{d_i hB} + O(h^{n+1})\,, \tag{4}$$

where k and n are the number of steps and the order of method respectively.

3. NEW SET OF CONDITIONS FOR FIFTH ORDER K-STEP SYMPLECTIC SCHEMES

3.1. *Description of the Procedure*

The determination of the coefficients c_i , d_i, is based on the expansion of the left-hand side of equation (4) in powers of h with $AB \neq BA$, i.e. on the formula:

$$S(h) = e^{h(A+B)} = 1 + h(A+B) + \frac{1}{2}h^2(A^2 + AB + BA + B^2) + ... \tag{5}$$

[3]See Wolfram Research Inc. `http://reference.wolfram.com`.
[4]`http://users.uop.gr/~simos/report_tselios_si5.pdf`.

Expanding the right hand side of (4) with $AB \neq BA$ it follows that:

$$\tilde{S}(h) = \prod_{i=1}^{k} e^{c_i hA} e^{d_i hB} = 1 + h\left(\sum_{i=1}^{k} c_i A + \sum_{i=1}^{k} d_i B\right) + \frac{1}{2}h^2\left[\left(\sum_{i=1}^{k} c_i\right)^2 A^2 + 2\sum_{i=1}^{k} d_i \sum_{j=1}^{i} c_j AB + 2\sum_{i=1}^{k} d_i \sum_{j=i+1}^{k} c_j BA + \left(\sum_{i=1}^{k} d_i\right)^2 B\right] + ... \qquad (6)$$

Demanding the two expressions (5) and (6) to agree up to h^n and assuming that the relations $(\sum_{i=1}^{k} c_i)^m = 1$ and $(\sum_{i=1}^{k} d_i)^m = 1$ with $m > 1$ hold, we obtain fifty-four equations for the fifth-order scheme (see for details Tselios & Simos 2011)[5].

Based on the analysis mentioned above, the equations for the k-step schemes till the fifth order are obtained. The conditions of their dependence are also determined.

Therefore, a new set of equations is produced. Based on this set of equations, one can develop a symplectic method of fifth-order solving those that are being linearly independent of each other.

3.2. *First order*

Based on the procedure described above and requiring the agreement of the relations (5) and (6) for the first power of h and for a k-step method (coefficients of A and B), the following relations hold:

$$f[1] = \sum_{i=1}^{k} c_i - 1\,, \qquad f[2] = \sum_{i=1}^{k} d_i - 1\,, \qquad (7)$$

which are linearly independent of each other.

3.3. *Second Order*

Requiring now the agreement of the relations (5) and (6) for the second power of h and for a k-step method (coefficients of AB and BA), the following relations hold:

$$f[3] = \sum_{i=1}^{k} d_i \sum_{j=1}^{i} c_j - \tfrac{1}{2!}\,, \qquad f[4] = \sum_{i=1}^{k} d_i \sum_{j=i+1}^{k} c_j - \tfrac{1}{2!}\,. \qquad (8)$$

From the above-mentioned functions it is easy to see that

$$1 - (1 + f[1])\,(1 + f[2]) + f[3] + f[4] = 0\,. \qquad (9)$$

For a second order method, the $f[1]$ and $f[2]$ of the first order should be zero; thus the following relation holds:

$$f[3] = -f[4]\,. \qquad (10)$$

Consequently, from the equations of the second-order it is sufficient to choose one of $f[3]$ or $f[4]$.

[5] http://users.uop.gr/~simos/report_tselios_si5.pdf.

3.4. *Third order*

Requiring the agreement of the relations (5) and (6) for the third power of h and for a k-step method (coefficients of A^2B, AB^2, BA^2, B^2A, ABA, BAB), the following relations hold:

$$\begin{aligned}
f[5] &= \tfrac{1}{2!}\sum_{i=1}^{k} d_i \left(\sum_{j=1}^{i} c_j\right)^2 - \tfrac{1}{3!}\,,\\
f[6] &= \tfrac{1}{2!}\sum_{i=1}^{k} c_i \left(\sum_{j=i}^{k} d_j\right)^2 - \tfrac{1}{3!}\,,\\
f[7] &= \tfrac{1}{2!}\sum_{i=1}^{k} d_i \left(\sum_{j=i+1}^{k} c_j\right)^2 - \tfrac{1}{3!}\,,\\
f[8] &= \tfrac{1}{2!}\sum_{i=2}^{k} c_i \left(\sum_{j=1}^{i-1} d_j\right)^2 - \tfrac{1}{3!}\,,\\
f[9] &= \sum_{i=1}^{k} c_i \sum_{j=i}^{k} d_j \sum_{l=j+1}^{k} c_l - \tfrac{1}{3!}\,,\\
f[10] &= \sum_{j=2}^{k} d_j \sum_{i=2}^{j} c_i \sum_{j=1}^{i-1} d_j - \tfrac{1}{3!}\,.
\end{aligned} \tag{11}$$

For the above-mentioned functions it has been found that

$$\begin{cases}
-(1+f[1])^2\,(1+f[2]) + (1+f[1])\,(1+2\,f[4]) + 2\,(f[5]-f[7]) = 0\,,\\
1-(1+f[1])^2\,(1+f[2]) + 2\,(f[5]+f[7]+f[9]) = 0\,,\\
1-(1+f[1])\,(1+f[2])^2 + 2\,(f[6]+f[8]+f[10]) = 0\,,\\
-\,(1+f[1])\,(1+f[2])^2 + (1+f[2])\,(1+2\,f[4]) + 2\,(f[6]-f[8]) = 0\,.
\end{cases} \tag{12}$$

For the third order method the $f[1]$,...,$f[4]$ of the second order should be zero; thus the following relations result:

$$\begin{aligned}
f[9] &= -2\,f[7] = -2f[5]\,,\\
f[10] &= -2\,f[8] = -2f[6]\,.
\end{aligned} \tag{13}$$

Therefore, from the equations of the third-order it is sufficient to choose one of $f[5]$ or $f[7]$ or $f[9]$ and one of $f[6]$ or $f[8]$ or $f[10]$.

3.5. *Fourth order*

Requiring the agreement of the relations (5) and (6) for the fourth power of h and for a k-step method (coefficients of A^3B, AB^3, BA^3,B^3A, A^2B^2, B^2A^2, A^2BA, AB^2A, ABA^2, B^2AB, BA^2B, BAB^2, $ABAB$, $BABA$),the following relations hold:

$$f[11] = \tfrac{1}{3!}\sum_{i=1}^{k} d_i \left(\sum_{j=1}^{i} c_j\right)^3 - \tfrac{1}{4!}\,,$$

$$f[12] = \tfrac{1}{3!}\sum_{i=1}^{k} c_i \left(\sum_{j=i}^{k} d_j\right)^3 - \tfrac{1}{4!}\,,$$

$$f[13] = \tfrac{1}{3!}\sum_{i=1}^{k} d_i \left(\sum_{j=i+1}^{k} c_j\right)^3 - \tfrac{1}{4!}\,,$$

$$f[14] = \tfrac{1}{3!}\sum_{i=2}^{k} c_i \left(\sum_{j=1}^{i-1} d_j\right)^3 - \tfrac{1}{4!}\,,$$

$$f[15] = \tfrac{1}{2!2!}\sum_{p=1}^{k}\sum_{j=p}^{k}\sum_{i=j}^{k}\sum_{m=i}^{k} c_p c_j a d_i d_m b - \tfrac{1}{4!},\quad a = \begin{cases} 1 & p=j\\ 2 & p\neq j\end{cases} \text{ and } \quad b = \begin{cases} 1 & i=m\\ 2 & i\neq m\end{cases}\,,$$

$$f[16] = \tfrac{1}{2!2!}\sum_{p=1}^{k-1}\sum_{j=p}^{k-1}\sum_{i=j+1}^{k}\sum_{m=i}^{k} d_p d_j a c_i c_m b - \tfrac{1}{4!}\quad a = \begin{cases} 1 & p=j\\ 2 & p\neq j\end{cases} \text{ and } \quad b = \begin{cases} 1 & i=m\\ 2 & i\neq m\end{cases}\,,$$

$$f[17]=\frac{1}{2!}\sum_{m=1}^{k}c_m\sum_{i=m}^{k}c_i\sum_{j=i}^{k}d_j\sum_{l=j+1}^{k}c_l+\frac{1}{2!}\sum_{m=1}^{k}c_m\sum_{i=m+1}^{k}c_i\sum_{j=i}^{k}d_j\sum_{l=j+1}^{k}c_l-\frac{1}{4!}\,,$$
$$f[18]=\frac{1}{2!}\sum_{j=1}^{k-1}c_j\sum_{i=j}^{k}d_i\sum_{m=i}^{k}d_m\sum_{l=m+1}^{k}c_l+\frac{1}{2!}\sum_{j=1}^{k-1}c_j\sum_{i=j}^{k}d_i\sum_{m=i+1}^{k}d_m\sum_{l=m+1}^{k}c_l-\frac{1}{4!}\,,$$
$$f[19]=\frac{1}{2!}\sum_{j=1}^{k-1}c_j\sum_{i=j}^{k}d_i\left(\sum_{j=i+1}^{k}c_j\right)^2-\frac{1}{4!}\,,$$
$$f[20]=\frac{1}{2!}\sum_{j=2}^{k}d_j\sum_{i=2}^{j}c_i\left(\sum_{j=1}^{i-1}d_j\right)^2-\frac{1}{4!}\,,$$
$$f[21]=\frac{1}{2!}\sum_{m=1}^{k}d_m\sum_{i=m+1}^{k}c_i\sum_{j=i}^{k}c_j\sum_{l=j}^{k}d_l+\frac{1}{2!}\sum_{m=1}^{k}d_m\sum_{i=m+1}^{k}c_i\sum_{j=i+1}^{k}c_j\sum_{l=j}^{k}d_l-\frac{1}{4!}\,,$$
$$f[22]=\frac{1}{2!}\sum_{j=1}^{k}d_j\sum_{i=j+1}^{k}c_i\left(\sum_{j=i}^{k}d_j\right)^2-\frac{1}{4!}\,,$$
$$f[23]=\sum_{m=1}^{k-1}c_m\sum_{j=m}^{k-1}d_j\sum_{i=j+1}^{k}c_i\sum_{l=i}^{k}d_l-\frac{1}{4!}\,,$$
$$f[24]=\sum_{m=1}^{k-2}d_m\sum_{j=m+1}^{k-1}c_j\sum_{i=j}^{k-1}d_i\sum_{l=i+1}^{k}c_l-\frac{1}{4!}\,.$$

For the above-mentioned functions it has been found that

$$\begin{cases} f[9]+3\,f[11]-f[19]=0\,,\\ -f[5]+3\,f[13]+f[19]=0\,,\\ f[5]+f[17]+f[19]=0\,,\\ -f[6]+3\,f[12]+f[22]=0\,,\\ -2\,f[6]+3\,f[14]-f[22]=0\,,\\ f[6]+f[20]+f[22]=0\,,\\ 2\,f[15]+f[23]=0\,,\\ 2\,f[16]+f[24]=0\,,\\ -f[6]+f[18]=0\,,\\ -f[5]+f[21]=0\,,\\ f[15]+f[16]+f[18]+f[21]+f[23]+f[24]=0\,. \end{cases} \tag{14}$$

For a fourth order method the functions $f[1]$,...,$f[10]$ of the third order should be zero; thus the following relations hold:

$$\begin{aligned} &f[13]=-f[11]=\tfrac{f[17]}{3}=-\tfrac{f[19]}{3}\,,\\ &f[14]=-f[12]=\tfrac{f[22]}{3}=-\tfrac{f[20]}{3}\,,\\ &f[24]=2f[15]=-2f[16]=-f[23]\,,\\ &f[18]=f[21]=0\,. \end{aligned} \tag{15}$$

Therefore, from the equations of the fourth-order it is sufficient to choose the $f[13]$, $f[14]$ and $f[24]$.

3.6. *Fifth order*

Requiring the agreement of the relations (5) and (6) for the fifth power of h and for a k-step method (coefficients of A^4B, AB^4, BA^4, B^4A, A^3B^2, A^2B^3, B^3A^2, B^2A^3, A^3BA, AB^3A, ABA^3, B^3AB, BA^3B, BAB^3, A^2B^2A, A^2BA^2, AB^2A^2, B^2A^2B, B^2AB^2, BA^2B^2, A^2BAB, AB^2AB, ABA^2B, $ABAB^2$, B^2ABA, BA^2BA, BAB^2A, $BABA^2$, $ABABA$, $BABAB$), the following relations hold:

$$f[25] = \frac{1}{4!}\sum_{i=1}^{k} d_i\left(\sum_{j=1}^{i} c_j\right)^4 - \frac{1}{5!}\,,$$

$$f[26] = \frac{1}{4!}\sum_{i=1}^{k} c_i\left(\sum_{j=i}^{k} d_j\right)^4 - \frac{1}{5!}\,,$$

$$f[27] = \frac{1}{4!}\sum_{i=1}^{k} d_i\left(\sum_{j=i+1}^{k} c_j\right)^4 - \frac{1}{5!}\,,$$

$$f[28] = \frac{1}{4!}\sum_{i=2}^{k} c_i\left(\sum_{j=1}^{i-1} d_j\right)^4 - \frac{1}{5!}\,,$$

$$f[29] = \frac{1}{3!2!}\sum_{i=1}^{k} d_i\left(\sum_{j=1}^{i} c_j\right)^3\sum_{m=i}^{k} d_m + \frac{1}{3!2!}\sum_{i=1}^{k} d_i\left(\sum_{j=1}^{i} c_j\right)^3\sum_{m=i+1}^{k} d_m - \frac{1}{5!}\,,$$

$$f[30] = \frac{1}{2!3!}\sum_{m=1}^{k} c_m\sum_{i=m}^{k} c_i\left(\sum_{j=i}^{k} d_j\right)^3 + \frac{1}{2!3!}\sum_{m=1}^{k} c_m\sum_{i=m+1}^{k} c_i\left(\sum_{j=i}^{k} d_j\right)^3 - \frac{1}{5!}\,,$$

$$f[31] = \frac{1}{3!2!}\sum_{i=2}^{k} c_i\sum_{l=i}^{k} c_l\left(\sum_{j=1}^{i-1} d_j\right)^3 + \frac{1}{3!2!}\sum_{i=2}^{k} c_i\sum_{l=i+1}^{k} c_l\left(\sum_{j=1}^{i-1} d_j\right)^3 - \frac{1}{5!}\,,$$

$$f[32] = \frac{1}{3!2!}\sum_{m=1}^{k} d_m\sum_{i=m}^{k} d_i\left(\sum_{j=i+1}^{k} c_j\right)^3 + \frac{1}{3!2!}\sum_{m=1}^{k} d_m\sum_{i=m+1}^{k} d_i\left(\sum_{j=i+1}^{k} c_j\right)^3 - \frac{1}{5!}\,,$$

$$f[33] = \frac{1}{3!}\sum_{m=2}^{k} c_m\sum_{i=1}^{m-1} d_i\left(\sum_{j=1}^{i} c_j\right)^3 - \frac{1}{5!}\,,$$

$$f[34] = \frac{1}{3!}\sum_{m=1}^{k} c_m\sum_{i=m+1}^{k} c_i\left(\sum_{j=m}^{i-1} d_j\right)^3 - \frac{1}{5!}\,,$$

$$f[35] = \frac{1}{3!}\sum_{m=1}^{k} c_m\sum_{i=m}^{k} d_i\left(\sum_{j=i+1}^{k} c_j\right)^3 - \frac{1}{5!}\,,$$

$$f[36] = \frac{1}{3!}\sum_{i=2}^{k} c_i\left(\sum_{j=1}^{i-1} d_j\right)^3\sum_{m=i}^{k} d_m - \frac{1}{5!}\,,$$

$$f[37] = \frac{1}{3!}\sum_{i=1}^{k} d_i\sum_{m=1}^{i-1} d_m\left(\sum_{j=m+1}^{i} c_j\right)^3 - \frac{1}{5!}\,,$$

$$f[38] = \frac{1}{3!}\sum_{m=1}^{k-1} d_m\sum_{i=m+1}^{k} c_i\left(\sum_{j=i}^{k} d_j\right)^3 - \frac{1}{5!}\,,$$

$$f[39] = \sum_{i=1}^{k-1}\sum_{j=i}^{k-1}\sum_{p=j}^{k-1}\sum_{q=p}^{k-1}\sum_{n=q+1}^{k} c_i c_j d_p d_q c_n ab - \frac{1}{5!}, \quad a = \begin{cases} \frac{1}{2!} & i=j \\ 1 & i\neq j \end{cases} \quad and \quad b = \begin{cases} \frac{1}{2!} & p=q \\ 1 & p\neq q \end{cases}\,,$$

$$f[40] = \sum_{i=1}^{k-1}\sum_{j=i}^{k-1}\sum_{p=j}^{k-1}\sum_{q=p+1}^{k}\sum_{n=q}^{k} c_i c_j d_p c_q c_n ab - \frac{1}{5!}, \quad a = \begin{cases} \frac{1}{2!} & i=j \\ 1 & i\neq j \end{cases} \quad and \quad b = \begin{cases} \frac{1}{2!} & q=n \\ 1 & q\neq n \end{cases}\,,$$

$$f[41] = \sum_{i=1}^{k-1}\sum_{j=i}^{k-1}\sum_{p=j}^{k-1}\sum_{q=p+1}^{k}\sum_{n=q}^{k} c_i d_j d_p c_q c_n ab - \frac{1}{5!}, \quad a = \begin{cases} \frac{1}{2!} & j=p \\ 1 & j\neq p \end{cases} \quad and \quad b = \begin{cases} \frac{1}{2!} & q=n \\ 1 & q\neq n \end{cases}\,,$$

$$f[42] = \sum_{i=1}^{k-1}\sum_{j=i}^{k-1}\sum_{p=j+1}^{k}\sum_{q=p}^{k}\sum_{n=q}^{k} d_i d_j c_p c_q d_n ab - \frac{1}{5!}, \quad a = \begin{cases} \frac{1}{2!} & i=j \\ 1 & i\neq j \end{cases} \quad and \quad b = \begin{cases} \frac{1}{2!} & p=q \\ 1 & p\neq q \end{cases}\,,$$

$$f[43] = \sum_{i=1}^{k-1}\sum_{j=i}^{k-1}\sum_{p=j+1}^{k}\sum_{q=p}^{k}\sum_{n=q}^{k} d_i d_j c_p d_q d_n ab - \frac{1}{5!}, \quad a = \begin{cases} \frac{1}{2!} & i=j \\ 1 & i\neq j \end{cases} \quad and \quad b = \begin{cases} \frac{1}{2!} & q=n \\ 1 & q\neq n \end{cases}\,,$$

$$f[44] = \sum_{i=1}^{k-1}\sum_{j=i+1}^{k}\sum_{p=j}^{k}\sum_{q=p}^{k}\sum_{n=q}^{k} d_i c_j c_p d_q d_n ab - \frac{1}{5!}, \quad a = \begin{cases} \frac{1}{2!} & j=p \\ 1 & j\neq p \end{cases} \quad and \quad b = \begin{cases} \frac{1}{2!} & q=n \\ 1 & q\neq n \end{cases}\,,$$

$$f[45] = -\frac{1}{5!} + \frac{1}{2!}\sum_{j=1}^{k-1} c_j\sum_{i=j}^{k-1} c_i\sum_{m=i}^{k-1} d_m\sum_{l=m+1}^{k} c_l\sum_{p=l}^{k} d_p + \frac{1}{2!}\sum_{j=1}^{k-1} c_j\sum_{i=j+1}^{k-1} c_i\sum_{m=i}^{k-1} d_m\sum_{l=m+1}^{k} c_l\sum_{p=l}^{k} d_p\,,$$

$$f[46] = -\frac{1}{5!} + \frac{1}{2!}\sum_{j=1}^{k-1} c_j \sum_{i=j}^{k-1} d_i \sum_{m=i}^{k-1} d_m \sum_{l=m+1}^{k} c_l \sum_{p=l}^{k} d_p + \frac{1}{2!}\sum_{j=1}^{k-1} c_j \sum_{i=j}^{k-1} d_i \sum_{m=i+1}^{k-1} d_m \sum_{l=m+1}^{k} c_l \sum_{p=l}^{k} d_p\,,$$

$$f[47] = -\frac{1}{5!} + \frac{1}{2!}\sum_{j=1}^{k-1} c_j \sum_{i=j}^{k-1} d_i \sum_{m=i+1}^{k} c_m \sum_{l=m}^{k} c_l \sum_{p=l}^{k} d_p + \frac{1}{2!}\sum_{j=1}^{k-1} c_j \sum_{i=j}^{k-1} d_i \sum_{m=i+1}^{k} c_m \sum_{l=m+1}^{k} c_l \sum_{p=l}^{k} d_p\,,$$

$$f[48] = -\frac{1}{5!} + \frac{1}{2!}\sum_{j=1}^{k-1} c_j \sum_{i=j}^{k-1} d_i \sum_{m=i+1}^{k} c_m \sum_{l=m}^{k} d_l \sum_{p=l}^{k} d_p + \frac{1}{2!}\sum_{j=1}^{k-1} c_j \sum_{i=j}^{k-1} d_i \sum_{m=i+1}^{k} c_m \sum_{l=m}^{k} d_l \sum_{p=l+1}^{k} d_p\,,$$

$$f[49] = -\frac{1}{5!} + \frac{1}{2!}\sum_{j=1}^{k-1} d_j \sum_{i=j}^{k-1} d_i \sum_{m=i+1}^{k} c_m \sum_{l=m}^{k} d_l \sum_{p=l+1}^{k} c_p + \frac{1}{2!}\sum_{j=1}^{k-1} d_j \sum_{i=j+1}^{k-1} d_i \sum_{m=i+1}^{k} c_m \sum_{l=m}^{k} d_l \sum_{p=l+1}^{k} c_p\,,$$

$$f[50] = -\frac{1}{5!} + \frac{1}{2!}\sum_{j=1}^{k-1} d_j \sum_{i=j+1}^{k-1} c_i \sum_{m=i}^{k} c_m \sum_{l=m}^{k} d_l \sum_{p=l+1}^{k} c_p + \frac{1}{2!}\sum_{j=1}^{k-1} d_j \sum_{i=j+1}^{k-1} c_i \sum_{m=i+1}^{k} c_m \sum_{l=m}^{k} d_l \sum_{p=l+1}^{k} c_p\,,$$

$$f[51] = -\frac{1}{5!} + \frac{1}{2!}\sum_{j=1}^{k-1} d_j \sum_{i=j+1}^{k-1} c_i \sum_{m=i}^{k} d_m \sum_{l=m}^{k} d_l \sum_{p=l+1}^{k} c_p + \frac{1}{2!}\sum_{j=1}^{k-1} d_j \sum_{i=j+1}^{k-1} c_i \sum_{m=i}^{k} d_m \sum_{l=m+1}^{k} d_l \sum_{p=l+1}^{k} c_p\,,$$

$$f[52] = -\frac{1}{5!} + \frac{1}{2!}\sum_{j=1}^{k-1} d_j \sum_{i=j+1}^{k-1} c_i \sum_{m=i}^{k} d_m \sum_{l=m+1}^{k} c_l \sum_{p=l}^{k} c_p + \frac{1}{2!}\sum_{j=1}^{k-1} d_j \sum_{i=j+1}^{k-1} c_i \sum_{m=i}^{k} d_m \sum_{l=m+1}^{k} c_l \sum_{p=l+1}^{k} c_p\,,$$

$$f[53] = -\frac{1}{5!} + \sum_{j=1}^{k-1} c_j \sum_{i=j}^{k-1} d_i \sum_{m=i+1}^{k} c_m \sum_{l=m}^{k-1} d_l \sum_{p=l+1}^{k} c_p\,,$$

$$f[54] = -\frac{1}{5!} + \sum_{j=1}^{k-1} d_j \sum_{i=j+1}^{k-1} c_i \sum_{m=i}^{k} d_m \sum_{l=m+1}^{k} c_l \sum_{p=l}^{k} d_p\,.$$

For the above-mentioned functions it has been found that

$$\begin{cases} f[25]+f[27]+f[33]+f[35]+f[40]=0\,,\\ \frac{-f[5]}{2}+3\,f[25]+f[27]+f[33]=0\,,\\ \frac{-f[5]}{2}+f[25]+3\,f[27]+f[35]=0\,,\\ -f[19]+3\,f[35]+2\,f[40]=0\,, \end{cases} \tag{16}$$

$$\begin{cases} f[26]+f[28]+f[36]+f[38]+f[43]=0\,,\\ \frac{-f[6]}{2}+f[26]+3\,f[28]+f[36]=0\,,\\ \frac{-f[6]}{2}+3\,f[26]+f[28]+f[38]=0\,,\\ -f[22]+3\,f[38]+2\,f[43]=0\,, \end{cases} \tag{17}$$

$$\begin{cases} f[29]+f[32]+f[37]+f[39]+f[41]+f[45]+f[47]+f[50]+f[52]+f[53]=0\,,\\ f[5]+\frac{f[6]}{2}-f[11]-f[15]+f[29]-f[32]=0\,,\\ \frac{-f[5]}{2}-\frac{f[6]}{2}-\frac{f[23]}{2}-f[39]+f[41]=0\,,\\ \frac{3\,f[5]}{2}-3\,f[11]+f[47]-f[50]=0\\ \frac{-5\,f[5]}{2}+\frac{f[10]}{2}+3\,f[11]+2\,f[15]+f[45]-f[52]=0\,,\\ \frac{-f[5]}{4}+\frac{f[11]}{2}+2\,f[29]-\frac{f[37]}{2}+f[45]=0\,,\\ \frac{f[5]}{6}-f[11]+f[37]+\frac{2\,f[47]}{3}=0\,,\\ \frac{f[5]}{2}+f[6]-2\,f[41]+f[45]+f[47]=0\,, \end{cases} \tag{18}$$

$$\begin{cases} f[30]+f[31]+f[34]+f[42]+f[44]+f[46]+f[48]+f[49]+f[51]+f[54]=0\,,\\ \frac{f[5]}{2}+f[6]-f[12]-f[15]+f[30]-f[31]=0\,,\\ -\frac{f[5]}{2}-\frac{f[6]}{2}+f[16]-f[42]+f[44]=0\,,\\ f[5]+\frac{f[10]}{4}+3\,f[12]-2\,f[16]+f[48]-f[49]=0\,,\\ \frac{f[6]}{2}-\frac{f[10]}{2}-3\,f[12]+f[46]-f[51]=0\,,\\ \frac{f[6]}{6}-f[12]+f[34]+\frac{2\,f[46]}{3}=0\,,\\ f[5]+\frac{f[6]}{2}-2\,f[44]+f[49]+f[51]=0\,,\\ -\frac{f[6]}{4}+\frac{f[14]}{2}+2\,f[31]-\frac{f[34]}{2}+f[49]=0\,. \end{cases} \tag{19}$$

TABLE 1

THE LINEARLY INDEPENDENT SYSTEM OF EQUATIONS FOR THE CONSTRUCTION OF A SYMPLECTIC INTEGRATOR OF FIFTH ORDER

Order	Equations	Number of equations
1	$f[1]=0, f[2]=0$	2
2	$f[3]=0$	3
3	$f[9]=0, f[10]=0$	5
4	$f[13]=0, f[14]=0, f[24]=0$	8
5	$f[25]=0, f[26]=0, f[29]=0, f[30]=0, f[53]=0, f[54]=0$	14

For the relations (16), (17), (18) and (19) the functions $f[1]$,...,$f[24]$ of the fourth order should be zero; thus the following relations hold:

$$f[25] = f[27] = -\frac{f[33]}{4} = -\frac{f[35]}{4} = \frac{f[40]}{6}\,, \tag{20}$$

$$f[26] = f[28] = -\frac{f[36]}{4} = -\frac{f[38]}{4} = \frac{f[43]}{6}\,, \tag{21}$$

$$\begin{aligned} f[37] &= -2f[29] + \tfrac{f[53]}{2}\,,\\ f[39] &= f[41] = -\tfrac{f[53]}{4}\,,\\ f[47] &= f[50] = 3f[29] - \tfrac{3f[53]}{4}\,,\\ f[45] &= f[52] = -3f[29] + \tfrac{f[53]}{4}\,,\\ f[32] &= f[29]\,, \end{aligned} \tag{22}$$

$$\begin{aligned} f[34] &= -2f[30] + \tfrac{f[54]}{2}\,,\\ f[42] &= f[44] = -\tfrac{f[54]}{4}\,,\\ f[46] &= f[51] = 3f[30] - \tfrac{3f[54]}{4}\,,\\ f[48] &= f[49] = -3f[30] + \tfrac{f[54]}{4}\,,\\ f[31] &= f[30]\,. \end{aligned} \tag{23}$$

Therefore, from the equations of the fifth-order it is sufficient to choose the $f[25]$, $f[26]$, $f[29]$, $f[30]$, $f[53]$ and $f[54]$.

Consequently, the following theorem was proved:

Theorem 1 *For the construction of a method of a fifth order and from the fifty four equations that should have been initially solved (and presented above), it is enough to solve only fourteen linearly independent equations, which are given in Table 1.*

4. CONSTRUCTION OF THE NEW FIFTH-ORDER METHOD

In this section we describe the development of the new proposed fifth-order method. Based on the above mentioned theory the new method is going to be a seven-step method, of the form (3), i.e.

$$
\begin{cases}
p_{j,1} = p_j^{\nu} - c_1 h(\frac{\partial V}{\partial q})_{q=q_j^{\nu}} \,, \\
q_{j,1} = q_j^{\nu} + d_1 h(\frac{\partial T}{\partial p})_{p=p_{j,1}} \,, \\
p_{j,2} = p_{j,1} - c_2 h(\frac{\partial V}{\partial q})_{q=q_{j,1}} \,, \\
q_{j,2} = q_{j,1} + d_2 h(\frac{\partial T}{\partial p})_{p=p_{j,2}} \,, \\
p_{j,3} = p_{j,2} - c_3 h(\frac{\partial V}{\partial q})_{q=q_{j,2}} \,, \\
q_{j,3} = q_{j,2} + d_3 h(\frac{\partial T}{\partial p})_{p=p_{j,3}} \,, \\
p_{j,4} = p_{j,3} - c_4 h(\frac{\partial V}{\partial q})_{q=q_{j,3}} \,, \\
q_{j,4} = q_{j,3} + d_4 h(\frac{\partial T}{\partial p})_{p=p_{j,4}} \,, \\
p_{j,5} = p_{j,4} - c_5 h(\frac{\partial V}{\partial q})_{q=q_{j,4}} \,, \\
q_{j,5} = q_{j,4} + d_5 h(\frac{\partial T}{\partial p})_{p=p_{j,5}} \,, \\
p_{j,6} = p_{j,5} - c_6 h(\frac{\partial V}{\partial q})_{q=q_{j,6}} \,, \\
q_{j,6} = q_{j,5} + d_6 h(\frac{\partial T}{\partial p})_{p=p_{j,6}} \,, \\
p_j^{\nu+1} = p_{j,6} - c_7 h(\frac{\partial V}{\partial q})_{q=q_{j,6}} \,, \\
q_j^{\nu+1} = q_{j,6} + d_7 h(\frac{\partial T}{\partial p})_{p=p_j^{\nu+1}} \,,
\end{cases}
\tag{24}
$$

with $j = 1, .., \nu$ where ν is the dimension of the vector p and q.

For the fifth order equations (Table 1), and for $k = 7$ (number of steps) we have fourteen equations and fourteen parameters. This set of equations can be solved numerically. Using the Newton or Levenberg-Marquardt method forty-six solutions for the fifth-order integrator have been obtained, (see for more details in Tselios & Simos 2011[6]). For internal computations 40-digits of precision are used.

For the study of the forty six produced schemes concerning error control, a similar procedure was followed (§ 3). Requiring the agreement of the relations (5) and (6) for the sixth power of h and for a k-step method, sixty two relations were found ($eq[1], ..., eq[62]$), (see for more details in Tselios & Simos 2011[7]).

We consider as error function the following:

$$
\text{FunError57} = \sqrt{eq[1]^2 + eq[2]^2 + ... + eq[62]^2} \,. \tag{25}
$$

After checking of all the forty six produced solutions, we have found that the scheme with the minimum error 0.1495161 is the following

$$
\begin{aligned}
c_1 &= 0.1125695844683471049731896848843277853938402393333314075493 \,, \\
c_2 &= 0.9238050290008374684475000700540644324911785274281141789991 \,, \\
c_3 &= -1.362064898669775624786044007840908597402026042205084284026 \,, \\
c_4 &= 0.980926531879316517259793318227431991923428491844523669724 \,, \\
c_5 &= 0.4009629674853713501479180258776577535775042274921907795 13 \,, \\
c_6 &= 0.345821780864741783378055242038676806930765132085822482512 \,, \\
c_7 &= -0.402020995028838599420412333241250172914690575978880873429 \,, \\
d_1 &= 0.369533888781149571850814500617016581067757439689950468 42 \,, \\
d_2 &= -0.032120004263046859169923904393901683486678946201463277409 \,, \\
d_3 &= -0.011978701020553903586622444048386301410473649207894475166 \,, \\
d_4 &= 0.512638174652696736042027856573955536074421583255396981 02 \,, \\
d_5 &= -0.334948298035883491345320878224434762455516821029015086331 \,, \\
d_6 &= 0.021856594741098449005512783774683495267598355789295971623 \,, \\
d_7 &= 0.475018345144539497203512085701067134942892037703729380 37 \,.
\end{aligned}
\tag{26}
$$

[6] http://users.uop.gr/~simos/report_tselios_si5.pdf.

[7] http://users.uop.gr/~simos/report_tselios_si5.pdf.

5. NUMERICAL EXAMPLES

The illustration of the efficiency of the new proposed method obtained in § 4 is examined by its application to the Two-body and Henon-Heiles problem. For comparison purposes the following methods are used:

- The four step-fourth order method developed by Yoshida (1990) which is indicated as YOS4.
- The eight step-six order[8] method developed by Yoshida (1990) which is indicated as YOS6.
- The new proposed method of seven step-fifth order which is indicated as SI5.

5.1. *Two-body problem*

The Hamiltonian of the two-body problem is given by

$$H = \frac{{p_1}^2}{2} + \frac{{p_2}^2}{2} - \frac{1}{\sqrt{q_1^2 + q_2^2}}\,, \tag{27}$$

where (q_1,q_2) are the conjugate coordinate and (p_1,p_2) are the conjugate momentum of the phase space. The equations of motion are

$$\begin{aligned} \dot{q_1} &= p_1\,, \\ \dot{q_2} &= p_2\,, \\ \dot{p_1} &= -\frac{q_1}{\sqrt{(q_1^2+q_2^2)^3}}\,, \\ \dot{p_2} &= -\frac{q_2}{\sqrt{(q_1^2+q_2^2)^3}}\,. \end{aligned} \tag{28}$$

The energy error is given by $E_{\rm error} = \frac{{p_1}^2}{2} + \frac{{p_2}^2}{2} - \frac{1}{\sqrt{q_1^2+q_2^2}}$, and the exact energy is $E_{\rm exact} = -0.5$.

The initial conditions are

$$p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \quad q_1(0) = 1-e, \quad q_2(0) = 0\,, \tag{29}$$

where the parameter e is the eccentricity.

In Figures 1, 2 and 3 we present for the same NFE (Number of Function Evaluations) and for different values of the eccentricity, time interval and step size the average energy error $\text{Err} = \log_{10}(E_{\rm average})$

$$E_{\rm average} = \frac{1}{\rm nsteps} \sum_{i=1}^{\rm nsteps} \|E_{\rm calculated} - E_{\rm exact}\|\,, \tag{30}$$

where $\text{nsteps} = t_{\max}/h$. In Figure 4 the position variables of the compared methods, for interval (0,1000), time step $\frac{1}{64}$ and eccentricity $e = 0.9$ are presented.

5.2. *Hénon-Heiles problem*

The Hamiltonian of the Henon-Heiles problem is given by

$$H = \frac{1}{2}({p_1}^2 + {p_2}^2) + \frac{1}{2}({q_1}^2 + {q_2}^2) + {q_1}^2 q_2 - \frac{1}{3} q_2^3\,, \tag{31}$$

[8]From the eight-steps sixth-order of Yoshida's methods it was selected for this comparison the one that gives the better results. For this method we have extended the precision of the given digits for its coefficients from 16 digits precision (that were proposed by Yoshida (1990) to 40 digits precision.

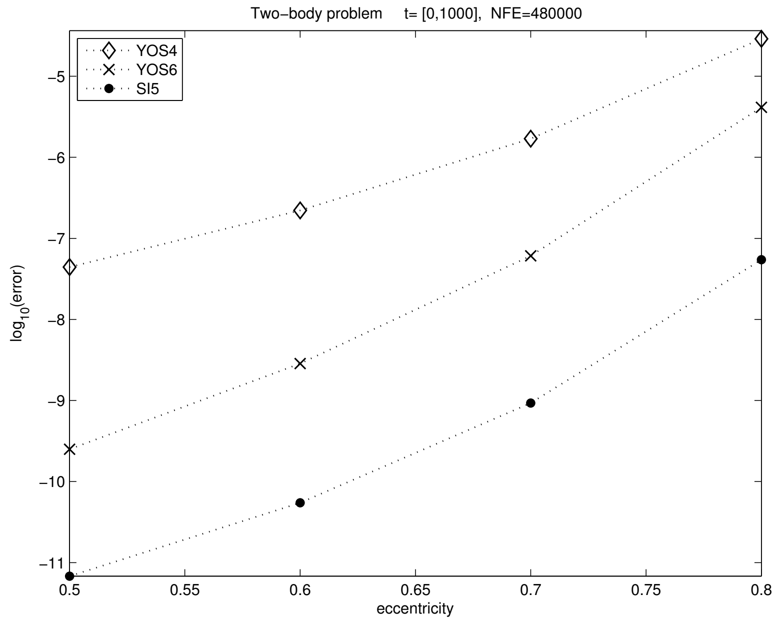

Fig. 1. Values of the average energy error for the eccentricity $e = 0.5$, 0.6, 0.7, 0.8 of the two body problem with time interval (0,1000) the same NFE=480000 and different step size h for each method. Methods used: (i) (diamonds) Yoshida [6] symplectic-scheme method of four step-fourth order with $h_4 = 8.3333e - 003$, (ii) (crosses) Yoshida [6] symplectic-scheme method of eight step-six order with $h_6 = 1.6667e-002$, (iii) (dots) New method with symplectic-scheme of seven step-fifth order with $h_5 = 1.4583e - 002$.

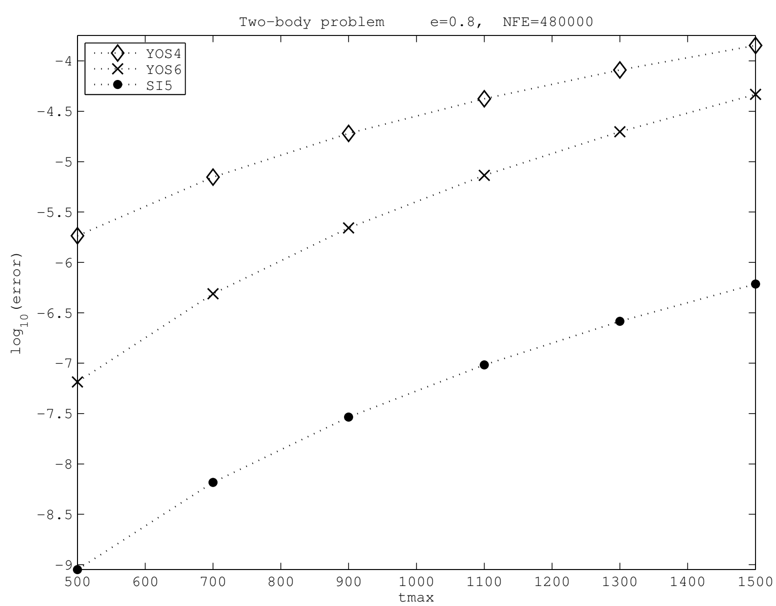

Fig. 2. Values of the average energy error of the two body problem, for time interval $(0, t_{\max})$, $t_{\max} = 500$,700,...,1500, eccentricity $e = 0.8$, the same NFE=480000 and different step size h for each method. Methods used: (i) (diamonds) Yoshida [6] symplectic-scheme method of four step-fourth order with $h_4 = t_{\max}$/nsteps4 where nsteps4=120000, (ii) (crosses) Yoshida [6] symplectic-scheme method of eight step-six order with $h_6 = 2h_4$, (iii) (dots) New Method with symplectic-scheme of seven step-fifth order with $h_5 = \frac{7}{4}h_4$.

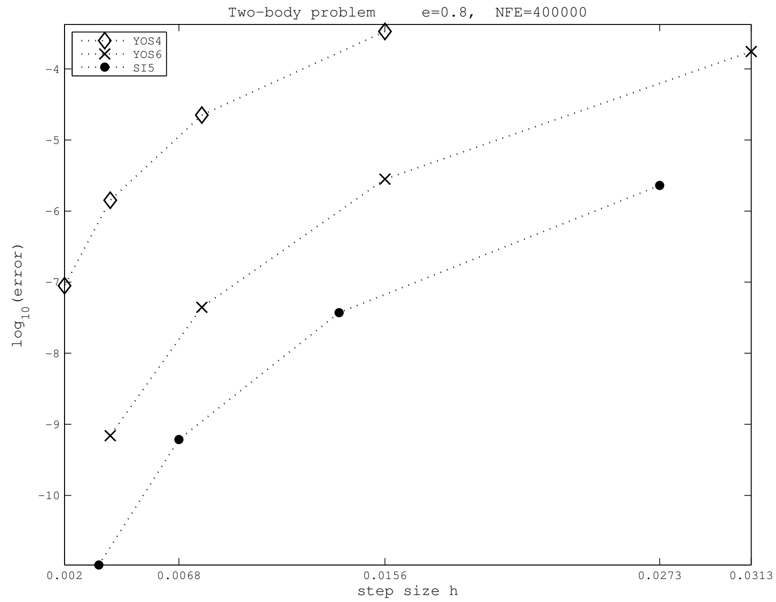

Fig. 3. Values of the average energy error of the two body problem, for $h_4 = 1/2^5$, $1/2^6$, $1/2^7$, $1/2^8$, eccentricity $e = 0.8$, the same NFE=400000 and time interval $(0, t_{\max})$, $t_{\max} = h_4 * \text{nsteps4}$, where nsteps4=100000. Methods used: (i) (diamonds) Yoshida [6] symplectic-scheme method of four step-fourth order with step size h_4, (ii) (crosses) Yoshida [6] symplectic-scheme method of eight step-six order with $h_6 = 2h_4$, (iii) (dots) New Method with symplectic-scheme of seven step-fifth order with $h_5 = \frac{7}{4}h_4$.

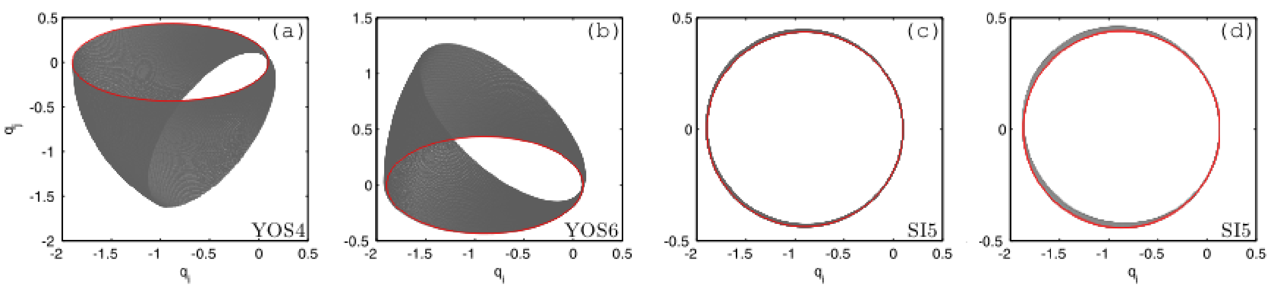

Fig. 4. The numerical solution of the two-body problem with interval (0,1000), eccentricity 0.9, the same NFE=480000 and different step size h for each method. The ellipse with red color is the exact solution. Methods used: (a) [YOS4] Yoshida [6] symplectic-scheme method of four step-fourth order with $h_4 = 8.3333e - 003$, (b) [YOS6] Yoshida [6] symplectic-scheme method of eight step-six order with $h_6 = 1.6667e - 002$, (c) [SI5] New Method with symplectic-scheme of seven step-fifth order with $h_5 = 1.4583e - 002$, (d) [SI5] New Method with symplectic-scheme of seven step-fifth order with $e = 0.9$, interval (0,1000), NFE=420000 and the same step size with [YOS6], $h = 1.6667e - 002$. The color figure can be viewed online.

where (q_1,q_2) are the conjugate coordinate and (p_1,p_2) are the conjugate momentum of the phase space. The equations of motion are

$$\dot{q_1} = p_1\,, \dot{q_2} = p_2\,, \dot{p_1} = -(q_1 + 2q_1q_2)\,, \dot{p_2} = -({q_1}^2 + q_2 - {q_2}^2)\,. \tag{32}$$

The initial conditions are $p_2(0) = 0$, $q_1(0) = 0.1$, $q_2(0) = 0$, and total energy $E = 0.15$. The $p_1(0)$ coordinate was determined from the following

$$p_1(0) = \sqrt{(2(E - V) - p_2(0)^2)}\,, \tag{33}$$

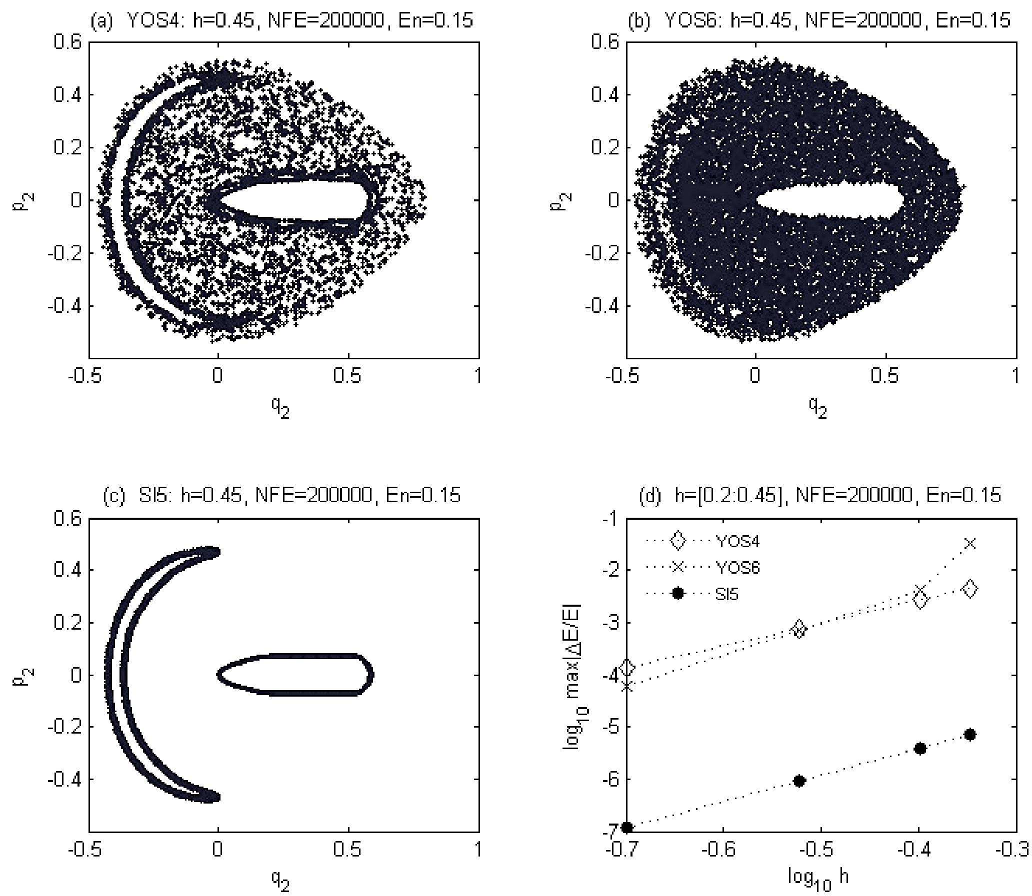

Fig. 5. (a),(b),(c) the Poincare surface of section of the (q_2,p_2) points in the $q_1 = 0$ plane with stepsize $h = 0.45$ and the same NFE=200000 for each method. Methods used: (i) [YOS4] Yoshida [6] symplectic-scheme method of four step-fourth order with $t_{\max} = 25000$, (ii) [YOS6] Yoshida [6] symplectic-scheme method of eight step-six order with $t_{\max} = 50000$, (iii) [SI5] New Method with symplectic-scheme of seven step-fifth order with $t_{\max} = 43750$. In (d) the energy loss for stepsize $h = 0.2, 0.3, 0.4, 0.45$. Both axes are logarithmic.

where V is the potential function

$$V = \frac{1}{2}({q_1}^2 + {q_2}^2) + {q_1}^2 q_2 - \frac{1}{3}q_2^3 \,. \tag{34}$$

In Figure 5d we present for the same NFE and for different values of the step size the energy loss Err=max$\| \frac{\Delta E}{E} \|$ and in Figures 5a,b,c the Poincare surface of section of the (q_2,p_2) points in the $q_1 = 0$ plane.

6. CONCLUSION

In this paper an optimized fifth algebraic order symplectic integrator was developed. The production of the new scheme was based on a new set of conditions for symplectic k-step schemes with order up to five. Based on this set, forty six symplectic seven-step methods of fifth algebraic order were obtained. The optimized fifth order symplectic integrator was defined using the minimum error. The numerical illustrations proved the efficiency of the new developed method compared with well known methods of the literature.

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