# Order 5 symplectic explicit Runge-Kutta Nyström methods

Lin-Yi Chou and P.W. Sharp*
Department of Mathematics, University of Auckland,
Private Bag 92019, Auckland, NEW ZEALAND.
linyi@scitec.auckland.ac.nz, sharp@scitec.auckland.ac.nz

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**Abstract**

Order five symplectic explicit Runge-Kutta Nyström methods of five stages are known to exist. However, these methods do not have free parameters with which to minimise the error coefficients. By adding one derivative evaluation per step, to give either a six-stage non-FSAL family or a seven-stage FSAL family of methods, two free parameters become available for the minimisation. This raises the possibility of improving the efficiency of order five methods despite the extra cost of taking a step.

We perform the minimisation of the two families to obtain an optimal method and then compare its performance with some published methods on the two-body problem for a range of eccentricities. These comparisons along with those based on the error coefficients show the new method is significantly more efficient than the five-stage methods. The numerical comparisons also suggest the new methods can be more efficient than some existing methods of other orders.

## 1 Introduction

Time-dependent processes such as those arising in mechanics and chemistry where dissipation is insignificant may often be modelled by a Hamiltonian system of ordinary differential equations of the form

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

where $' \equiv d/dt$ and $H : \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathbb{R}$ is sufficiently smooth.

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A one step numerical method for (1) is called symplectic if it preserves the symplectic structure of the space of variables $(p, q)$, thus reproducing the main qualitative property of the solution. Numerical experiments have shown symplectic methods can be more efficient than non-symplectic methods for long intervals of integration.

Symplectic Runge-Kutta methods are necessarily implicit. However for separable Hamiltonians (those of the form $H(q,p) = T(p) + V(q)$), explicit Runge-Kutta Nyström (ERKN) methods can be symplectic if the coefficients of the method satisfy certain conditions.

Okunbor and Skeel [5] investigated families of symplectic ERKN methods which used one, two and three stages. Calvo and Sanz-Serna in [1], [2] and [3] presented and tested a five-stage, order four method with minimised (principal) error coefficients. The method re-uses the last stage as the first stage of the next step (FSAL) so that only four derivations evaluations are required on each step, except for the first step. In [4] Calvo and Sanz-Serna presented a 13-stage, order seven FSAL method with minimised error coefficients. Okunbar and Skeel [6] investigated the existence of order five and six methods. They performed an extensive numerical search and found four individual five-stage, order five methods. They conjectured there were no six-stage methods of order six and through a numerical search obtained 16 individual seven-stage order six methods.

For five-stage, order five methods, there are ten order conditions to satisfy and ten coefficients to satisfy these conditions. Hence, there are no coefficients available with which to minimise the error coefficients. If one stage is added, and the order is kept at five, two coefficients become available, but this is at the expense of increasing (by one) the number of derivative evaluations required to take a step.

This trade-off between decreasing the error and increasing the cost for each step raises the interesting question of whether the introduction of the sixth stage will lead to a gain or loss in efficiency, where efficiency is measured by the number of derivative evaluations required to achieve a prescribed global error.

It is this question we address.

# 2 The methods

## 2.1 Definitions

When a Hamiltonian is separable, (1) can be written as

$$y'' = f(y), \tag{2}$$

where $f : \mathbb{R}^n \mapsto \mathbb{R}^n$.

The ERKN methods we consider use $s$-stages and generate order $p$ approximations $y_i$ and $y'_i$ to $y(x_i)$ and $y'(x_i)$ respectively, $i = 1, 2, \ldots$, according to

$$y_i \quad = \quad y_{i-1} + hy'_{i-1} + h^2 \sum_{j=1}^{s} b_j f_j, \tag{3}$$

$$y'_i = y'_{i-1} + h \sum_{j=1}^{s} b'_j f_j, \tag{4}$$

where $h = x_i - x_{i-1}$, the prime in $b'_j$ denotes the derivative formula and not the derivative of $b_j$, and

$$f_j = f(x_{i-1} + c_j h, y_{i-1} + c_j h y'_{i-1} + h^2 \sum_{k=1}^{j-1} a_{jk} f_k), \quad j = 1, \ldots, s.$$

In all the methods we consider, the $b_j$ are given by

$$b_j = (1 - c_j) b'_j, \quad j = 1, \ldots, s. \tag{5}$$

For an ERKN method to be symplectic, the $a_{jk}$ must satisfy

$$a_{jk} = (c_j - c_k) b'_k, \quad k = 1, \ldots, j-1, \quad j = 2, \ldots, s. \tag{6}$$

Hence once $c_j$, $b_j$, $j = 1, \ldots, s$ are known, the remaining coefficients of a symplectic ERKN are known.

For a method to be FSAL, its coefficients must satisfy $c_1 = 0$, $c_s = 1$ and

$$a_{sj} = b_j, \quad j = 1, \ldots, s-1. \tag{7}$$

If $c_1 = 0$ and $c_s = 1$ and the method is symplectic, (7) is automatically satisfied.

We decided against using the simplifying assumptions

$$\frac{c_j}{2} = \sum_{k=1}^{j-1} a_{jk}, \quad j = 2, \ldots, s,$$

because these led to a net reduction in the number of free parameters available for minimising the error coefficients.

In the remainder of this paper the term 'method' will mean 'symplectic method' unless stated otherwise.

## 2.2 Six-stage, order five non-FSAL methods

There are 13 order conditions up to an including order five. However, three of these order conditions are dependent on the remainder (see for example [6]). This means, since we have twelve coefficients available ($c_j$, $b_j$, $j = 1, \ldots, 6$) with a six-stage non-FSAL ERKN method, we can take two coefficients as free parameters and solve for the others. We found it convenient to take $c_5$ and $c_6$ as the free parameters.

Five of the 10 order conditions to satisfy are the quadrature conditions

$$\sum_{j=1}^{s} b_j c_j^k = (k+1)^{-1}, \quad k = 0, \ldots, 4, \tag{8}$$

where we take $0^0 = 1$ and $0^k = 0$, $k > 0$. Conditions (8) are easily solved for $b'_1, \ldots, b'_5$ in terms of the $c$ and $b'_6$.

The next condition we solve is

$$\sum_{j=2}^{6} b'_j \sum_{k=1}^{j-1} a_{jk} = \frac{1}{6}. \tag{9}$$

When the expressions for $b'_1, \ldots, b'_5$ found from solving (8) are substituted into (9), the equation becomes a quadratic in $b'_6$. This is solved to give $b'_6$ and hence the other $b'$ in terms of the $c$.

This leaves the following equations to satisfy, where summations are performed over $i$ and $j$

$$b_i c_i a_{ij} = \frac{1}{8}, \quad b_i c_i^2 a_{ij} = \frac{1}{10}, \quad b_i c_i a_{ij} c_j = \frac{1}{30}, \quad b_i (a_{ij})^2 = \frac{1}{20}. \tag{10}$$

When the expressions for the $b'$ are substituted into the above equations, the equations become complicated functions of the $c$. Even with the help of MAPLE we were unable to solve these equations algebraically and resorted to a numerical approach.

We first attempted to use a non-interactive grid method consisting of an outer and inner grid. The outer grid was over $c_5$ and $c_6$ (the free parameters) and was used to minimise the euclidean norm of the order six error coefficients for the solution and derivative formulae. The inner grid was over $c_1$, $c_2$, $c_3$ and $c_4$ (the unknowns) and was used to generate initial estimates of the solutions of (10). For each point on the inner grid, we used the package HYBRD (obtained from NETLIB) to solve (10). If a solution was found, we evaluated the norm of the error coefficients and updated our minimum and minimiser if required. As in [4], a solution was accepted only if $-1.5 \leq c_j, b_j \leq 1.5$, $j = 1, \ldots, 6$.

Although the above grid method produced tangible results after several days of CPU time, there was much duplication of effort because HYBRD would converge to the same solution from different points on the inner grid. In addition, the method had the air of brute force, something we found unappealing.

We then attempted an interactive grid-search consisting of just the outer grid. By keeping a history stack of the previously converged solutions, we were able to, after gaining some experience, make rapid progress in the minimisation.

At intermediate points during the grid search, we tested the best method we had and compared its performance with published methods on a set of test problems. On a number of occasions we found the norm of the error coefficients significantly over-estimated the efficiency of the new method. On other occasions what we thought was a significant decrease in the norm led to little or no improvement in the efficiency.

We were unable to ascertain the reason for this sometimes poor correlation between the predicted and actual performance.

## 2.3 Seven-stage, order five FSAL methods

The derivation and minimisation of seven-stage, order five FSAL methods is similar to that for the six-stage non-FSAL methods, the main difference being $b'_7$ is now a free parameter in place of $c_1$. We used the interactive grid method and found through our testing at intermediate points of the search that methods from the FSAL family were more efficient than those from the non-FSAL family.

Using a grid size of 0.01 for $c_5$ and $c_6$, the best method we found had $c_j, b_j,\ j = 1, 7$ as follows

$$
\begin{array}{lcllcl}
c_1 &=& 0.0000000000000000E+00 & c_2 &=& 0.2179621390175646E+00 \\
c_3 &=& 0.4424703708255242E+00 & c_4 &=& 0.1478460559438898E+01 \\
c_5 &=& 0.3400000000000000E+00 & c_6 &=& 0.7000000000000000E+00 \\
c_7 &=& 0.1000000000000000E+01 & & & \\
b'_1 &=& 0.6281213570268329E-01 & b'_2 &=& 0.3788983131252575E+00 \\
b'_3 &=& 0.2754528515261340E+00 & b'_4 &=& -0.1585299574780513E-02 \\
b'_5 &=& -0.1785704038527618E+00 & b'_6 &=& 0.3479995834198831E+00 \\
b'_7 &=& 0.1149928196535844E+00 & & &
\end{array}
$$

The remaining coefficients can be found using (5) and (6). The error in satisfying the order conditions is less than $3 \times 10^{-16}$.

The euclidean norm of the order six error coefficients for the solution and derivative formula is $4.0 \times 10^{-4}$ and $4.1 \times 10^{-4}$ respectively. The corresponding norms for the four, five-stage order five methods given in [6] range from $1.7 \times 10^{-2}$ to $2.4 \times 10^{-2}$ for the solution formula and $3.3 \times 10^{-2}$ to $4.3 \times 10^{-2}$ for the derivative formula.

An estimate of the relative efficiency of the new method and those in [6] can be obtained by assuming the global error varies as the fifth root of the norms. After scaling by the number of derivative evaluations performed on a step, the predicted gain in efficiency is 100 to 110 percent i.e. the new method is predicted to be twice as efficient as those in [6].

# 3 Numerical experiments

We tested the new method on a set of test problems for different intervals of integration and compared its performance with the order four method in [3], the order seven method in [4] and one of the order five methods from [6] (we chose the fourth method in Table 1, any of the other methods in the table could have been used without materially affecting our conclusions). Here we present a summary of the test results from the two-body problem

$$x'' = -\frac{x}{r^3}, \quad x(0) = 1 - e, \quad x'(0) = 0, \tag{11}$$

$$y'' = -\frac{y}{r^3}, \quad y(0) = 0, \quad y'(0) = \sqrt{\frac{1+e}{1-e}}, \tag{12}$$

for a range of eccentricities ($e$).

Figures 1, 2 and 3 give the log-log graphs of the number of derivative evaluations against the norm of the end-point global error for $e = 0.3, 0.5$ and $0.7$. The interval of integration is 10,000 and we used stepsizes of $2^{-i}$, $i = 2, \ldots, 7$.

We consider Figures 1 and 2 first. The new method is more efficient than the five-stage one which means it was advantageous to use an extra stage to form the method. The gain in efficiency is approximately a factor of two which agrees well with the gain predicted using the norm of the error coefficients. We also observe the new method is more efficient than the order four and order seven methods, except at small global errors for $e = 0.3$.

The results in Figure 3 provide a caveat to the above conclusions. The new method has retain much of its efficiency relative to the five-stage, order five method except at large global errors, but the order four method is now of similar efficiency to the new method at large global errors.

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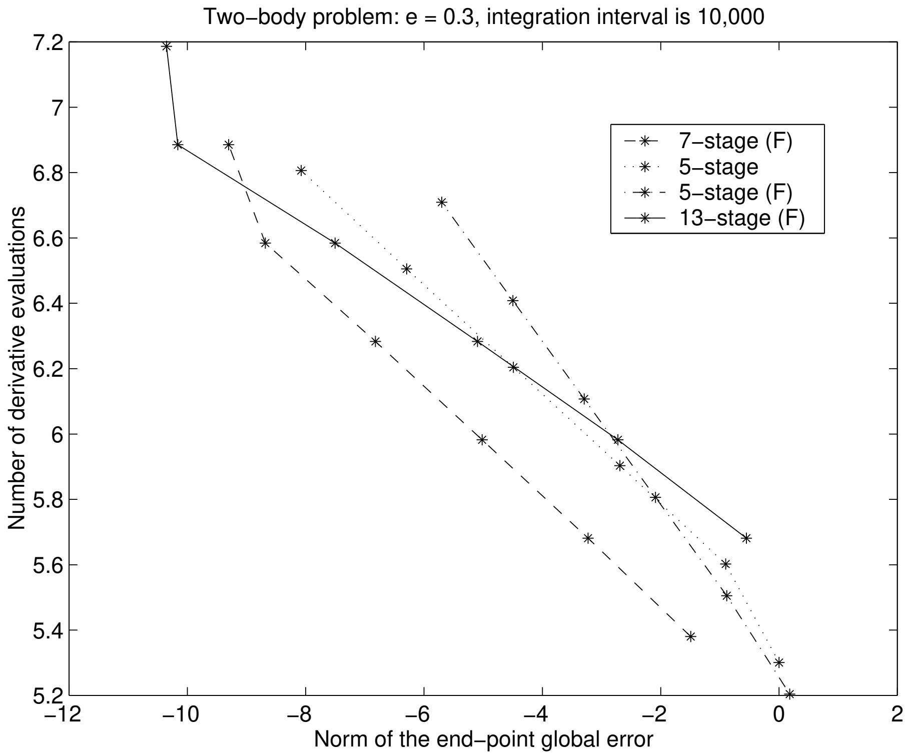


Figure 1: Base 10 log-log graph of the number of derivative evaluations against the norm of the end-point global error for the two-body problem with $e = 0.3$ and an integration interval of 10,000. New method - dashed line, order five method of Okunbor and Skeel - dotted line, order four method of Calvo and Sanz-Serna - dash-dot line, order seven method of Calvo and Sanz-Serna - solid line.

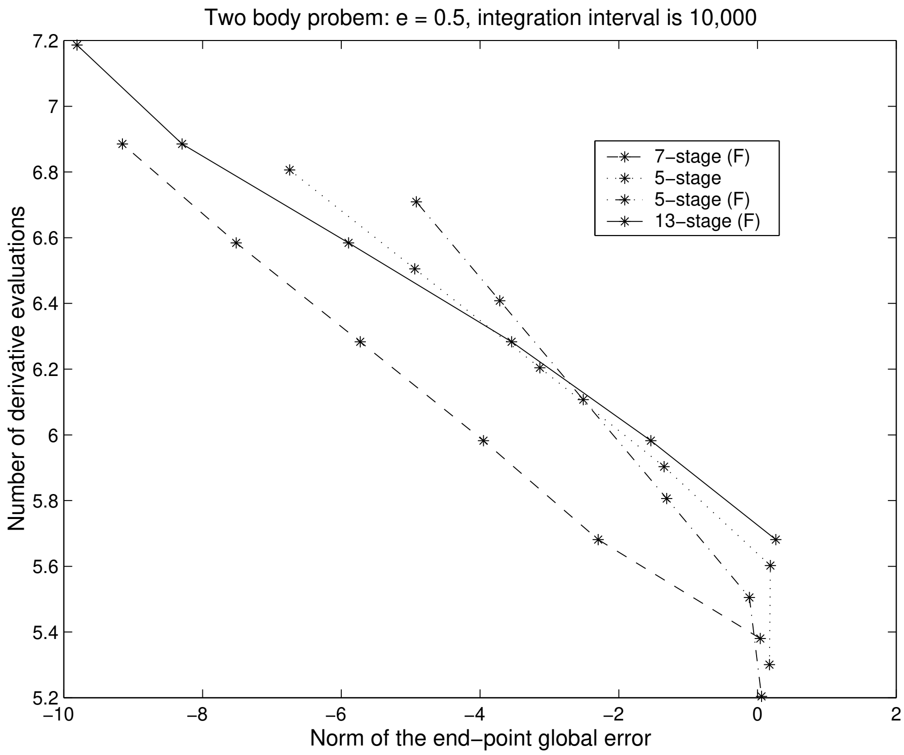


Figure 2: Base 10 log-log graph of the number of derivative evaluations against the norm of the end-point global error for the two-body problem with $e = 0.5$ and an integration interval of 10,000. New method - dashed line, order five method of Okunbor and Skeel - dotted line, order four method of Calvo and Sanz-Serna - dash-dot line, order seven method of Calvo and Sanz-Serna - solid line.

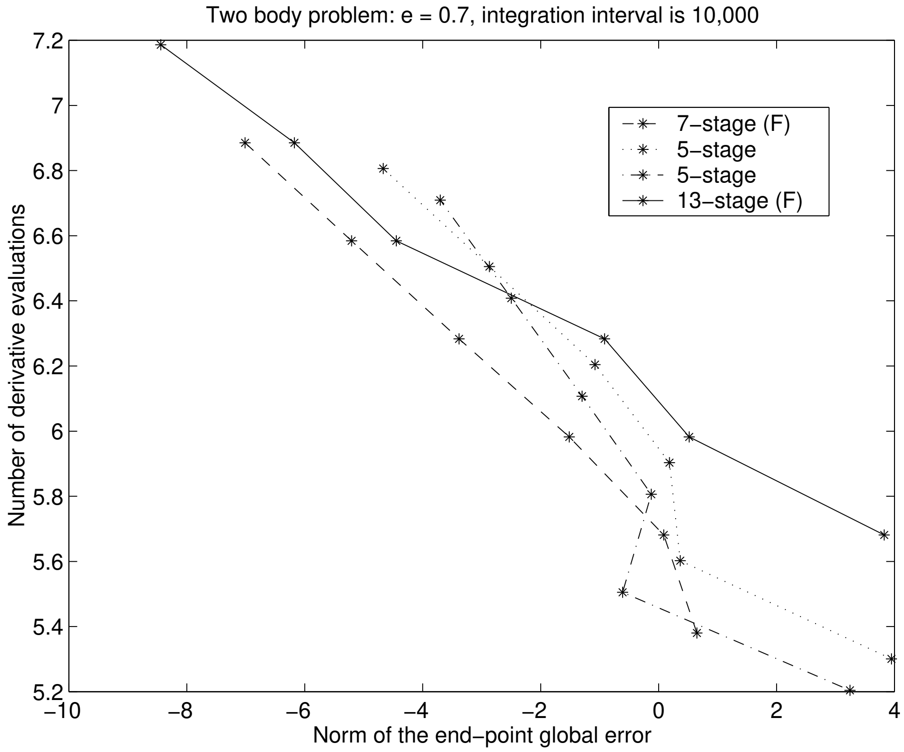


Figure 3: Base 10 log-log graph of the number of derivative evaluations against the norm of the end-point global error for the two-body problem with $e = 0.7$ and an integration interval of 10,000. Ne w method - dashed line, order five method of Okunbor and Skeel - dotted line, order four method of Calvo and San z-Serna - dash-dot line, order seven method of Calvo and Sanz-Serna - solid line.