

On fitted modifications of Runge–Kutta–Nyström Pairs

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Abstract

Modification of only four coefficients of the standard Runge–Kutta–Nyström pairs is enough for producing a method of the same orders that integrates exactly the harmonic oscillator as model problem. These new coefficients are $O(\lambda^2)$ perturbations of the initial ones, with λ the frequency of the problem. Theoretical investigation for the possibilities of order reduction is given. Numerical results over standard pairs of orders 6(4) and 8(6) justify our efforts.

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1. Introduction

Explicit Runge–Kutta–Nyström pairs are widely used for the numerical solution of the initial value problem

$$y'' = f(x, y), \quad y(x_0) = y_0 \in \mathbb{R}^m, \quad y'(x_0) = y_0' \in \mathbb{R}^m, \quad x \in [x_0, x_e]$$

where $f : \mathbb{R} \times \mathbb{R}^m \mapsto \mathbb{R}^m$. We usually use the extended Butcher tableau [3] of the method's coefficients :

$$\begin{array}{c|c} c & A \\ \hline & b, b' \\ & \hat{b}, \hat{b}' \end{array}$$

to present the RKN pair. In such a tableau $b^T, \hat{b}^T, b'^T, \hat{b}'^T, c \in \mathbb{R}^s$ and $A \in \mathbb{R}^{s \times s}$ is strictly lower triangular.

Such a method implementing the following formulae:

$$y_{n+1} = y_n + hy'_n + h_n^2 \sum_{i=1}^s b_i f_{ni}$$

and

$$\hat{y}_{n+1} = y_n + hy'_n + h_n^2 \sum_{i=1}^s \hat{b}_i f_{ni}$$

advances the solution from x_n to $x_{n+1} = x_n + h_n$ computing at each step approximations y_{n+1}, \hat{y}_{n+1} to $y(x_{n+1})$ of orders p and q respectively, with $q < p$.

It also produces two approximations y'_{n+1}, \hat{y}'_{n+1} to $y'(x_{n+1})$ of orders p and q , given by

$$y'_{n+1} = y'_n + h \sum_{i=1}^s b'_i f_{ni}$$

and

$$\hat{y}'_{n+1} = y'_n + h \sum_{i=1}^s \hat{b}'_i f_{ni}.$$

Here

$$f_{ni} = f(x_n + c_i h_n, y_n + h_n \sum_{j=1}^{i-1} a_{ij} f_{nj}) \in \mathbb{R}^m$$

for $i = 1, 2, \dots, s \geq p$. These embedded form methods (called RKN $p(q)$) are implemented with variable step-sizes as we can obtain an estimate

$$u_{n+1} = \max(\|y_{n+1} - \hat{y}_{n+1}\|_\infty, \|y'_{n+1} - \hat{y}'_{n+1}\|_\infty)$$

of the local truncation error of the q order formula. If this error estimation is less than a requested tolerance TOL it is common to apply the step-size control algorithm

$$h_{n+1} = 0.9h_n \cdot \left(\frac{TOL}{h^{p-q-1}u_{n+1}}\right)^{1/p}, \quad (1)$$

to compute the next step-size. If it is not, we use the same formula to recompute the current step. See [18] for more details on the implementation of these type of step size policies.

2. Oscillatory Problems

Many authors have dealt in the past with the numerical integration of oscillatory problems [1, 2, 6, 7, 8, 9, 11, 13, 16]. Traditionally we consider as test problem the harmonic oscillator:

$$y'' = -\lambda^2 y, \quad y(0) = 1, \quad y'(0) = i\lambda, \quad \lambda \in R \quad (2)$$

with exact solution $\bar{y} = e^{i\lambda x}$

When (2) is solved numerically by a Nyström method, the following recursive relation is obtained

$$Y_{n+1} = R(z_n) Y_n, \quad z_n = -v_n^2, \quad v_n = \lambda h_n$$

where $Y_n = [y_n, h_n y'_n]^T$ and after discharging indexes n we have,

$$R(z) = \begin{vmatrix} 1 + zb(I - zA)^{-1}e & 1 + zb(I - zA)^{-1}c \\ zb'(I - zA)^{-1}e & 1 + zb'(I - zA)^{-1}c \end{vmatrix}$$

where $e = [1, 1, \dots, 1]^T \in \mathbb{R}^s$.

The theoretical solution $\bar{Y}_n = \bar{Y}(x_n) = [\bar{y}(x_n), h_n \bar{y}'(x_n)]^T$ satisfies the recursive relation

$$\bar{Y}_{n+1} = \bar{R}(v_n) \bar{Y}_n$$

where, discharging indexes again

$$\bar{R}(v) = \begin{vmatrix} \cos v & \frac{\sin v}{v} \\ -v \sin v & \cos v \end{vmatrix}$$

Since $\det \bar{R}(v) \equiv 1$ and $\text{trace}[\bar{R}(v)] = 2 \cos(v)$, we may also require

$$\begin{aligned} \det R(v) &\equiv 1 \\ \text{trace}[R(v)] &= 2 \cos(v) \end{aligned} \tag{3}$$

Equations (3) can be solved for two of the parameters of an existing pair with respect to v . Thus we get a pair with phase error and amplification error of infinite order.

Alternatively, we chose to match all the entries of matrices R and \bar{R} . We require,

$$\begin{aligned} 1 + zb(I - zA)^{-1}e &= \cos v, \\ 1 + zb(I - zA)^{-1}c &= \frac{\sin v}{v}, \\ zb'(I - zA)^{-1}e &= -v \sin v, \\ 1 + zb'(I - zA)^{-1}c &= \cos v \end{aligned} \tag{4}$$

For the latter equations the following Theorem holds.

Theorem: *A Runge-Kutta-Nyström method of even algebraic order p , when modified by perturbing four coefficients in order to satisfy Equations (4), retain its order if the altered coefficients are chosen from the following sets*

- i) $a_{j_1, j_2}, a_{j_3, j_4}, a_{j_5, j_6}, a_{j_7, j_8}$
- ii) $a_{j_1, j_2}, a_{j_3, j_4}, b_{j_5}, b_{j_6}$
- iii) $a_{j_1, j_2}, a_{j_3, j_4}, c_{j_5}, c_{j_6}$
- iv) $a_{j_1, j_2}, b_{j_3}, b_{j_4}, c_{j_5}$
- v) $a_{j_1, j_2}, b_{j_3}, b_{j_4}, b'_{j_5}$
- vi) $a_{j_1, j_2}, b_{j_3}, c_{j_4}, c_{j_5}$
- vii) $a_{j_1, j_2}, c_{j_3}, c_{j_4}, b'_{j_5}$
- viii) $a_{j_1, j_2}, c_{j_3}, b'_{j_4}, b'_{j_5}$
- ix) $b_{j_1}, b_{j_2}, c_{j_3}, b'_{j_4}$
- x) $b_{j_1}, b_{j_2}, b'_{j_3}, b'_{j_4}$
- xi) $b_{j_1}, c_{j_2}, c_{j_3}, b'_{j_4}$
- xii) $b_{j_1}, c_{j_2}, b'_{j_3}, b'_{j_4}$

for proper values of the indices.

Proof: Suppose that a p -th order method shares coefficients b , b' , A and c . The truncations errors are

$$h^2\left(b e - \frac{1}{2}\right) T_1^{(2)} + h^3\left(b c - \frac{1}{6}\right) T_1^{(3)} + h^4\left(\left(b A e - \frac{1}{24}\right) T_1^{(4)} + \frac{1}{2}\left(b c^2 - \frac{1}{12}\right) T_2^{(4)}\right) + \dots$$

for $y(x)$ and

$$h(b'e - 1) T_1'^{(2)} + h^2(b'c - \frac{1}{2}) T_1'^{(3)} + h^3\left(\left(b' A e - \frac{1}{6}\right) T_1'^{(4)} + \frac{1}{2}\left(b' c^2 - \frac{1}{3}\right) T_2'^{(4)}\right) + \dots$$

for $y'(x)$. The various T and T' 's are elementary differentials, e.g. $T_1^{(2)} = f$, $T_1^{(3)} = \frac{\theta f}{\theta y} y'$, etc. See [17] for details.

Thus for a p -th order method all the coefficients of the elementary differentials of orders less or equal p are nullified.

Expanding equations (4) we get the equivalent expressions [14],

$$1 - v^2 b e + v^4 b A e - v^6 b A^2 e \pm \dots = 1 - \frac{1}{2} v^2 + \frac{1}{24} v^4 - \frac{1}{720} v^6 \pm \dots \quad (5)$$

$$1 - v^2bc + v^4bAc - v^6bA^2c \pm \dots = v - \frac{1}{6}v^2 + \frac{1}{120}v^4 - \frac{1}{5040}v^6 \pm \dots \quad (6)$$

$$-v^2b'e + v^4b'Ae - v^6b'A^2e \pm \dots = -v^2 + \frac{1}{6}v^4 - \frac{1}{120}v^6 \pm \dots \quad (7)$$

$$1 - v^2b'c + v^4b'Ac - v^6b'A^2c \pm \dots = 1 - \frac{1}{2}v^2 + \frac{1}{24}v^4 - \frac{1}{720}v^6 \pm \dots \quad (8)$$

Let's choose the 10th set and alter the coefficients b_{j_1} , b_{j_2} , b'_{j_3} , b'_{j_4} in order to satisfy equations (5-8). Then b_{j_1} , b_{j_2} are used for solving (5-6) while b'_{j_3} , b'_{j_4} are used for solving (7-8). For the altered coefficients we observe that

$$\tilde{b}_{j_1} = b_{j_1} + v^{p-2}\tilde{b}_{j_1,p-2} + v^p\tilde{b}_{j_1,p} + O(v^{p+2}), \quad (9)$$

$$\tilde{b}_{j_2} = b_{j_2} - v^{p-2}\tilde{b}_{j_2,p-2} + v^p\tilde{b}_{j_2,p} + O(v^{p+2})$$

with $\tilde{b}_{j_2,p-2} = \tilde{b}_{j_1,p-2}$.

Now, the truncation error coefficients for the modified method \tilde{b} , \tilde{b}' , A , c become:

$$\tilde{b}e - 1/2, \tilde{b}c - \frac{1}{6}, \text{ or } \tilde{b}'e - 1, \tilde{b}c - \frac{1}{2}, \tilde{b}Ae - \frac{1}{6} \text{ etc.} \quad (10)$$

Thus, since $be = \frac{1}{2}$, $v = O(h)$ and the symmetrical coefficients of v^{p-2} ,

$$h^2(\tilde{b}e - \frac{1}{2}) = h^2(be - \frac{1}{2}) + O(h^{p+2}) = O(h^{p+2})$$

and the order is attained while the perturbations summed into higher order truncation error coefficients.

We proceed and verify that the order is attained for the other expressions of (10). These five truncation error coefficients are generally enough to check if there is order reduction.

If in the contrary choose a little different set, presumedly b_{j_1} , a_{j_2,j_3} , b'_{j_4} , b'_{j_5} then we have to solve (5-6) for b_{j_1} and a_{j_2,j_3} . But now only (9) holds and the symmetric cancelations withdrawn

$$h^2(\tilde{b}e - \frac{1}{2}) = O(h^p)$$

losing an order of accuracy. \square

Remarks:

- r1: There are cases where choosing from the sets suggested by Theorem we can't satisfy equations (4). e.g. selecting a_{21} , a_{31} , a_{51} and a_{61} of set (i).

- r2: There is a possibility where the underlying method has coefficients that cancel the order reduction. e.g. a pair of orders 6(4) from the families studied in [4, 12] with free coefficients $c_2 = 0.1261321989868105$, $c_3 = 0.3$ and $c_4 = 0.7$ can be altered for a_{32} , a_{54} , b'_1 and b'_2 without losing accuracy.
- r3: For a fourth order method with three stages there might be cases where selecting to perturb a coefficient from matrix A is equivalent to choose a coefficient from vector c . This is due to the almost obligatory assumption $Ae = \frac{c^2}{2}$ that leaves only one free coefficient from matrix A .
- r4: For methods of odd order it seems that we can't choose from sets (vii) and (viii) of the Theorem. On the other hand it seems that there are three more sets we can choose from. Namely (i) a_{j_1, j_2} , a_{j_3, j_4} , a_{j_5, j_6} , b_{j_7} (ii) a_{j_1, j_2} , a_{j_3, j_4} , a_{j_5, j_6} , c_{j_7} and (iii) a_{j_1, j_2} , a_{j_3, j_4} , b_{j_5} , c_{j_6} .

3. The new modified pairs

First we consider the standard in the literature five stages pair RKN6(4)6FM, of orders 6(4) given in [4]. For this pair $s = 6$ but the First Stage of each step is the same As the Last stage of the previous step (FSAL). After solving (4) with respect to the coefficients a_{41} , c_4 , b'_1 and b'_2 we get the following expressions.

$$\tilde{a}_{41} = -\frac{7(80v^{10} - 18447v^8 + 928840v^6 - 7895250v^4 + 392040000v^2 + 784080000 \cos(v) - 784080000)}{726000v^4 (16v^2 - 2475)}$$

$$\tilde{c}_4 = -\frac{7(80v^9 - 7887v^7 + 268620v^5 + 2450250v^3 + 39204000v - 39204000 \sin(v))}{36300v^3 (16v^2 - 2475)}$$

$$\tilde{b}'_1 = -\frac{45696(8v^4 - 2025v^2 + 123750)v \cos(v) + 50575v^7 - 1761938v^5 + 714(16v^6 - 10115v^4 + 1308000v^2 - 19800000) \sin(v) - 340239600v^3 + 8482320000v}{171360v^3 (16v^2 - 2475)}$$

$$\tilde{b}'_2 = \frac{5(-8352v(16v^2 - 2475) \cos(v) - 696(16v^4 - 3075v^2 + 99000) \sin(v) + v(725v^6 + 14560v^4 - 3253968v^2 + 48232800))}{4176v^3(16v^2 - 2475)}$$

It was proved in the tests bellow that choosing variable nodes does not affect numerical integration.

Next we consider the widely known eighth stages pair RKN8(6)9FM of orders 8(6) given in [5]. For this pair $s = 9$ but FSAL device is used also. After solving (4) with respect to the coefficients b_1 , b_3 , b'_1 and b'_3 we get lengthy expressions.

Traditionally, Taylor expansion for small values of v is used instead. But higher order pairs take long steps and $v \gg 0$. Thus we present an L_∞ rational approximation in the interval $[0, 2]$ with polynomials of degree 10. This technique minimizes the overhead of the computation.

This evaluation was done with Maple. After solving equations-(4) and stored a coefficient, say b_1 , in variable `b1` we may proceed typing:

```

b1 := (-986767/1323+5400/v^2+4691849*v^2/158760-319*v^4/560
+21654739*v^6/3407611200-1728497*v^8/34076112000
-45353*v^10/525745728000-cos(v)+600*cos(v)/v^2-6000*sin(v)/v^3
+30*sin(v)/v-v*sin(v)/40)/(-600+v^2):
Digits := 40:
with(numapprox):
sol := fnormal(minimax(b1, v=-2..2, [10,11], 1, 'err'), 16, 10^(-15))

```

Thus we avoid odd powers of v that appear with very small coefficients anyway. Then equating with 1 the coefficient of v^0 in the denominator and rationalizing, we get the following expressions.

$$\tilde{b}_1 = \frac{\frac{1217v^{10}}{2079620646580} + \frac{11855v^8}{2261768522667} + \frac{23570v^6}{200841030927} - \frac{26995v^4}{154026538486} + \frac{925561v^2}{22751070275} + \frac{223}{7938}}{-\frac{12v^{10}}{386770807809059} + \frac{710v^8}{43498281621349} - \frac{2664v^6}{1261916628107} - \frac{121082v^4}{19408214259} + \frac{2790782v^2}{1927154205} + 1}$$

$$\tilde{b}_3 = \frac{-\frac{3331v^{10}}{4674896130199} + \frac{20913v^8}{8116925922179} - \frac{71872v^6}{1075558492505} + \frac{1869757v^4}{233794887226} + \frac{5960727v^2}{4602738985} + \frac{1175}{8064}}{\frac{63v^{10}}{3722810505670} + \frac{41844v^8}{18411745608205} + \frac{228613v^6}{658414161700} + \frac{2750667v^4}{50115862199} + \frac{28078817v^2}{3159244729} + 1}$$

$$\tilde{b}'_1 = \frac{\frac{64226v^{10}}{19202155671093} + \frac{68273v^8}{1113213675447} + \frac{51019v^6}{2946631237705} + \frac{607639v^4}{295630594047} + \frac{5352649v^2}{19953503370} + \frac{223}{7938}}{\frac{1927v^{10}}{33001272660911} + \frac{28213v^8}{6032275339068} + \frac{275547v^6}{447078002948} + \frac{1786672v^4}{24419813093} + \frac{200835295v^2}{21032175657} + 1}$$

$$\tilde{b}'_3 = \frac{-\frac{15776v^{10}}{3944678694119} - \frac{25517v^8}{958459236473} + \frac{657562v^6}{2063404581135} + \frac{1033436v^4}{32818992581} + \frac{13599389v^2}{4952695777} + \frac{5875}{36288}}{\frac{3560v^{10}}{16185312784333} + \frac{41556v^8}{2332506697979} + \frac{1014416v^6}{515357512531} + \frac{11469927v^4}{58972175785} + \frac{13318803v^2}{785294017} + 1}$$

When $v = 0$ we get the conventional pair RKN8(6)9FM. The denominator of the rational form is always far from zero for $v \in [0, 2]$. The differences from the actual values are always under the limits of double precision arithmetic.

Even with rational forms the overhead may be significant for small problems. A way around this is to tabulate and exclusively use the coefficients for fixed values of v , e.g. for $v = 0, 0.05, 0.1, \dots, 1.95, 2$. Then we may admit an 2.5% increase in the cost or translate it to loss of less than 0.1 digits in accuracy. This is acceptable since as we'll see in the numerical tests our gain is much greater.

4. Numerical tests

We tested the new pairs on three standard problems from the literature [10, 19].

1. Bessel equation

equation:

$$y'' = \left(-100 + \frac{1}{4x^2}\right) y, \quad x \in [1, 100]$$

initial values:

$$y(1) = J_0(10x), \quad y'(1) = -0.5576953439142885$$

exact solution:

$$y(x) = \sqrt{x}J_0(10x)$$

2. Inhomogeneous equation

equation:

$$y'' = -100y + 99 \sin x, \quad x \in [0, 100]$$

initial values:

$$y(0) = 1, \quad y'(0) = 11$$

exact solution:

$$y(x) = \cos 10x + \sin 10x + \sin x$$

3. Duffing equation

equation:

$$y'' = -y - y^3 + \frac{1}{500} \cos(1.01x), \quad x \in [0, 100]$$

initial values:

$$y(0) = 0.2004267280699011, \quad y'(0) = 0$$

approximate exact solution:

$$y(x) \approx \begin{aligned} &0.2001794775368452 \cos(1.01t) - 2.469461432611 \cdot 10^{-4} \cos(3.03t) \\ &- 3.040149839 \cdot 10^{-7} \cos(5.05t) - 3.743495 \cdot 10^{-10} \cos(7.07t) \\ &- 4.609 \cdot 10^{-13} \cos(9.09t) - 6 \cdot 10^{-16} \cos(11.11t) \end{aligned} \quad (11)$$

For the first two problems $\lambda = 10$ was used while $\lambda = 1.01$ was chosen for the Duffing Equation.

In Tables 1-3 we recorded for each tolerance $TOL = 10^{-3}, 10^{-4}, \dots, 10^{-9}$ the function evaluations (stages) used and the end-point global error observed for the conventional pair RKN6(4)6FM and its fitted modification RKN6(4)f.

It is clear that the fitted modification is much more efficient. Even for the case of the strongly non-linear problem the gain of almost one digit is remarkable. For the latter problem we presented above an approximation of enhanced accuracy (11) for recording the errors at stringent tolerances.

As expected by the Theorem in section 2, the variable nodes do not affect the efficiency of RKN6(4)f. All tested problems involve the independent variable x , thus we have a strong indication for this.

In the derivation of the new fitted RKN pairs only the higher order formula of each pair is modified. However, the lower order formula of each pair can be also modified so that it integrates exactly the harmonic oscillator. We tried modifying again RKN6(4)f, satisfying proper modification of equations

Table 1: Results of 6(4) pairs for the Bessel equation

TOL	RKN6(4)f		RKN6(4)6FM		RKN6(4)6ff	
	stages	error	stages	error	stages	error
10^{-3}	3166	$10^{-6.60}$	3166	$10^{-2.45}$	781	$10^{-2.02}$
10^{-4}	6316	$10^{-8.49}$	6316	$10^{-3.86}$	1141	$10^{-3.15}$
10^{-5}	8641	$10^{-8.85}$	8671	$10^{-4.60}$	1261	$10^{-4.92}$
10^{-6}	12086	$10^{-9.90}$	12086	$10^{-5.55}$	2036	$10^{-5.65}$
10^{-7}	16476	$10^{-10.83}$	16556	$10^{-6.51}$	2456	$10^{-7.10}$
10^{-8}	23111	$10^{-11.75}$	23066	$10^{-7.51}$	3471	$10^{-8.01}$
10^{-9}	32821	$10^{-12.52}$	32831	$10^{-8.59}$	5256	$10^{-8.72}$

(4) for \hat{b}_1 , \hat{b}_2 , \hat{b}'_1 and \hat{b}'_2 . This choice does not affect coefficients used by the higher order formula and thus we avoid the possibility of order reduction.

The new pair is named RKN6(4)ff. The results over the test problems are listed in the right columns of Tables 1-3. It seems that this error estimation is too optimistic and the step size control has to be adapted in order to retain tolerance proportionality. The efficiency curves are not tuned to agree with those of standard pairs. As the problem is closest to the model (2) then step-size control algorithm (1) becomes inappropriate. Further analysis is needed and some other parameters have to be included in (1) along with algebraic order p .

In Tables 4-6 we recorded for each tolerance $TOL = 10^{-5}, 10^{-7}, \dots, 10^{-10}$ the function evaluations and the end-point global error observed for the conventional pair RKN8(6)9FM and its fitted modification RKN8(6)f.

Again it is clear that the fitted modification is much more efficient. Even for the case of the strongly non-linear problem the gain of almost one digit is remarkable. In the past much effort was put for constructing higher order pairs for less profit [15]. The pair need sometimes to be applied for quadruple precision in order to get the correct number of accuracy digits. The performance for Bessel and Inhomogeneous was restrained for high tolerances due to roundoff errors.

Table 2: Results of 6(4) pairs for the Inhomogeneous problem

TOL	RKN6(4)f		RKN6(4)6FM		RKN6(4)6ff	
	stages	error	stages	error	stages	error
10^{-3}	5701	$10^{-6.54}$	5631	$10^{-2.78}$	1776	$10^{-3.01}$
10^{-4}	7956	$10^{-7.40}$	7966	$10^{-3.77}$	2746	$10^{-4.80}$
10^{-5}	11121	$10^{-8.55}$	11141	$10^{-4.53}$	4021	$10^{-5.51}$
10^{-6}	15441	$10^{-9.57}$	15451	$10^{-5.51}$	5811	$10^{-7.34}$
10^{-7}	21216	$10^{-10.30}$	21246	$10^{-6.48}$	8511	$10^{-8.67}$
10^{-8}	30531	$10^{-11.19}$	30446	$10^{-7.56}$	12316	$10^{-9.84}$
10^{-9}	43131	$10^{-12.20}$	43061	$10^{-8.64}$	18046	$10^{-10.36}$

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References

- [1] G. V. Berghe and M. Van Daele, Exponentially-fitted Numerov methods, *J. Comput. Appl. Math.*, **200** 140-153 (2007)
- [2] G. V. Berghe and M. Van Daele, Symplectic exponentially-fitted four-stage RungeKutta methods of the Gauss type, *Numer. Algorithms*, **56** 591-608 (2011)
- [3] J. C. Butcher, *The Numerical Analysis of Ordinary Differential Equations*, John Wiley & Sons Inc., New York (1987).
- [4] J. R. Dormand, M. E. El-Mikkawy, and P. J. Prince, Families of Runge–Kutta–Nyström formulae, *IMA J. Num. Analysis* **7** (1987), 235–250.
- [5] J. R. Dormand, M. E. El-Mikkawy, and P. J. Prince, High order embedded Runge–Kutta–Nyström formulae, *IMA J. Num. Analysis* **7** (1987), 423–430.

Table 3: Results of 6(4) pairs for the Duffing equation

TOL	RKN6(4)f		RKN6(4)6FM		RKN6(4)6ff	
	stages	error	stages	error	stages	error
10^{-3}	451	$10^{-3.18}$	441	$10^{-2.96}$	311	$10^{-4.27}$
10^{-4}	626	$10^{-5.45}$	626	$10^{-4.66}$	416	$10^{-4.19}$
10^{-5}	761	$10^{-6.49}$	761	$10^{-5.48}$	596	$10^{-5.46}$
10^{-6}	996	$10^{-7.88}$	996	$10^{-6.54}$	931	$10^{-6.70}$
10^{-7}	1456	$10^{-8.66}$	1456	$10^{-7.63}$	1186	$10^{-8.12}$
10^{-8}	2136	$10^{-9.53}$	2136	$10^{-8.66}$	1721	$10^{-8.92}$
10^{-9}	3131	$10^{-10.54}$	3131	$10^{-9.69}$	2521	$10^{-9.62}$

Table 4: Results of 8(6) pairs for the Bessel equation

TOL	RKN8(6)f		RKN8(6)9FM	
	stages	error	stages	error
10^{-5}	7465	$10^{-8.86}$	7513	$10^{-4.71}$
10^{-6}	9649	$10^{-10.08}$	9649	$10^{-5.87}$
10^{-7}	11569	$10^{-11.45}$	11569	$10^{-7.05}$
10^{-8}	15225	$10^{-12.90}$	15225	$10^{-8.32}$
10^{-9}	20305	$10^{-13.90}$	20305	$10^{-9.69}$
10^{-10}	27089	$10^{-14.20}$	27089	$10^{-11.00}$

- [6] J.M. Franco, Exponentially fitted explicit Runge-Kutta-Nyström methods, *J. Comput. Appl. Math.*, **167**, 1-19 (2004).
- [7] J.M. Franco and I. Gomez, Some procedures for the construction of high-order exponentially fitted Runge-Kutta-Nyström methods of explicit type, *Comput. Phys. Commun.*, **184**, 1310-1321 (2013).
- [8] Z. Kalogiratou, Th. Monovasilis and T.E. Simos, Symplectic Runge-Kutta-Nyström Methods with Phase-Lag Order Six and Infinity, *AIP Conf. Proc.*, **1281** 694-697 (2010).
- [9] Z. Kalogiratou and T.E. Simos, Construction of Trigonometrically and

Table 5: Results of 8(6) pairs for the Inhomogeneous problem

TOL	RKN8(6)f		RKN8(6)9FM	
	stages	error	stages	error
10^{-5}	9177	$10^{-9.88}$	9177	$10^{-4.82}$
10^{-6}	11385	$10^{-10.95}$	11385	$10^{-6.00}$
10^{-7}	14297	$10^{-11.82}$	14297	$10^{-7.24}$
10^{-8}	19081	$10^{-12.10}$	19081	$10^{-8.58}$
10^{-9}	25449	$10^{-12.68}$	25449	$10^{-10.27}$
10^{-10}	33945	$10^{-13.20}$	33945	$10^{-11.00}$

Table 6: Results of 8(6) pairs for the Duffing equation

TOL	RKN8(6)f		RKN8(6)9FM	
	stages	error	stages	error
10^{-5}	801	$10^{-6.84}$	801	$10^{-7.81}$
10^{-6}	1201	$10^{-8.79}$	1201	$10^{-7.71}$
10^{-7}	1633	$10^{-9.31}$	1633	$10^{-8.73}$
10^{-8}	2105	$10^{-10.38}$	2105	$10^{-9.65}$
10^{-9}	2681	$10^{-11.60}$	2681	$10^{-10.58}$
10^{-10}	3297	$10^{-12.34}$	3297	$10^{-11.58}$

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- [10] G Papageorgiou, Ch. Tsitouras and I. Th. Famelis, Explicit Numerov type methods for second order IVPs with oscillating solutions, *Int. J. Mod. Phys. C*, **12**, 657-666 (2001).
- [11] G. Papageorgiou, Ch. Tsitouras and S. N. Papakostas, Runge-Kutta pairs for periodic initial value problems, *Computing*, **51**, 151-163 (1993).
- [12] S. N. Papakostas and Ch. Tsitouras, High Phase-Lag-Order Runge–Kutta and Nyström Pairs, *SIAM J. Sci. Comput.*, **21**, 747-763 (1999).

- [13] T. E. Simos, Exponentially-fitted Runge-Kutta-Nystrom method for the numerical solution of initial-value problems with oscillating solutions, *Appl. Math. Lett.*, **15**, 217-225 (2002).
- [14] Ch. Tsitouras, High order zero dissipative Runge-Kutta-Nyström methods, *J. Comput. Appl. Math.*, **95**, 157-161 (1998).
- [15] Ch. Tsitouras, Optimized explicit Runge-Kutta pair of orders 9(8), *Appl. Numer. Math.*, **38**, 123-134 (2001).
- [16] Ch. Tsitouras, Explicit eighth order two-step methods with nine stages for integrating oscillatory problems, *Int. J. Modern Phys. C*, **17**, 861-876 (2006).
- [17] Ch. Tsitouras and I. Th. Famelis, Symbolic derivation of Runge-Kutta-Nyström order conditions, *J. Math. Chem.*, **46**, 896-912 (2009).
- [18] Ch. Tsitouras and S. N. Papakostas, Cheap Error Estimation for Runge-Kutta pairs, *SIAM J. Sci. Comput.*, **20**, 2067-2088 (1999).
- [19] Ch. Tsitouras and T. E. Simos, High algebraic, high phase-lag order embedded Numerov-type methods for oscillatory problems, *Appl. Math. Comput.*, **131**, 201-211 (2002).