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An improved class of generalized Runge-Kutta-Nyström methods for special second order differential equations

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We propose a new family of explicit methods of order four with two evaluations per step, for the numerical integration of special second order differential equations given by $y'' = f(y)$. These two-stage formulas can be seen as a generalization of the explicit two-stage Runge-Kutta-Nyström methods, providing better order and stability results. We will show that it is possible to obtain methods that are more efficient than the classical Runge-Kutta-Nyström one-step methods with the same number of evaluations per step, specially when highly oscillatory problems are considered. Some numerical experiments are discussed in order to show the good performance of the new schemes.

Key words: Generalized Runge-Kutta-Nyström Methods, Oscillatory problems, Numerical Experiments.

1 Introduction.

Many differential equations which appear in practice are special second order differential equations given by $y'' = f(x, y)$. It is a common practice to transform this equation into a first order differential equation of doubled dimension by considering the vector (y, y') as the new variable. In order to solve numerically the system, one can for instance apply a Runge-Kutta method to the first order differential system. However, a real improvement can be achieved

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by applying some special methods to equation $y'' = f(x, y)$ directly. For example Störmer [12] developed accurate and simple multistep methods for this special second order differential equations that are more efficient than the classical Runge-Kutta and multistep methods. A similar situation also holds for Nyström [9] one-step methods. For more details [6] is a good reference.

In this work we will obtain new methods for the problem

$$y'' = f(y), \quad y(x_0) = y_0, \quad y'(x_0) = z_0, \quad f : \mathbb{R} \rightarrow \mathbb{R}.$$

Second order scalar autonomous ODEs are of little interest in current applications. However, we begin studying this kind of problems because most of the work can be easily extended to a more general situation. In fact, it is possible to generalize many of our methods so that they can be applied to some special systems.

In [2,1,3,5] we developed similar methods for first order ODEs given by $y' = f(y)$ and in [4] we investigated a generalization of the schemes that applies to some special systems.

2 A first example.

We begin considering, as a first example, an explicit two stage method of order four that gives the exact solution (except for round-off errors) when applied to equation $y'' = -\alpha y + \beta$ with $\alpha > 0, \beta \in \mathbb{R}$. This method is given by

$$\begin{aligned} y_{n+1} &= y_n + h \left(\left(\frac{\cos \sqrt{-s} - 1}{s} \right) (k_1 - c_1 s y'_n) + \left(\frac{\text{sen} \sqrt{-s}}{\sqrt{-s}} \right) y'_n \right), \\ y'_{n+1} &= y'_n + \left((\cos \sqrt{-s} - 1) y'_n + \left(\frac{\text{sen} \sqrt{-s}}{\sqrt{-s}} \right) (k_1 - c_1 s y'_n) \right), \end{aligned} \quad (1)$$

where

$$\begin{aligned} k_1 &= hf(y_n + hc_1 y'_n), \quad k_2 = hf(y_n + h(c_2 y'_n + d_2 k_1)), \\ s &= \frac{k_2 - k_1}{(c_2 - c_1) y'_n + d_2 k_1}, \end{aligned} \quad (2)$$

and parameters take the values

$$c_1 = \frac{3 - \sqrt{3}}{6}, \quad c_2 = \frac{3 + \sqrt{3}}{6}, \quad d_2 = \frac{\sqrt{3}}{6}. \quad (3)$$

This method performs well when applied to oscillatory problems. It is easy to show that the term s can be seen as an approximation to $h^2 f_y$. In fact we have that $s = h^2 f_y(y_n) + O(h^3)$.

In order to show the good performance of this method we will consider the following nonlinear oscillatory problem (a perturbed oscillator)

$$y'' = -\alpha y + \varepsilon y^3, \quad y(x_0) = 1, \quad y'(x_0) = 0, \quad (4)$$

taking different values for the parameters α and ε , and different step sizes. We have integrated this problem with fixed step size, using our method and the three stage Nyström method of order four given in [6], pp. 285. In the following two tables we show the errors measured with respect to the first integral $(\alpha y^2 + y'^2)/2 - \varepsilon y^4/4$ (because the exact solution is not available). We take $x_{end} = 1000$ and $\varepsilon = 10^{-3}$ in all cases.

Table 1
Errors for our method.

error	$h = 0.1$	$h = 0.05$	$h = 0.025$	$h = 0.0125$
$\alpha = 100$	$5.912D - 03$	$2.103D - 04$	$6.751D - 06$	$2.122D - 07$
$\alpha = 10$	$6.912D - 06$	$2.192D - 07$	$6.930D - 09$	$2.203D - 10$
$\alpha = 1$	$6.621D - 09$	$1.970D - 10$	$5.520D - 12$	$1.296D - 13$

Table 2
Errors for Nyström's method.

error	$h = 0.1$	$h = 0.05$	$h = 0.025$	$h = 0.0125$
$\alpha = 100$	$5.000D + 01$	$3.309D + 01$	$1.667D + 00$	$5.294D - 02$
$\alpha = 10$	$1.701D - 01$	$5.389D - 03$	$1.675D - 04$	$5.172D - 06$
$\alpha = 1$	$1.715D - 05$	$5.307D - 07$	$1.626D - 08$	$4.882D - 10$

Note that our method performs better than Nyström's method in all numerical experiments, specially when we take $\alpha \gg 1$, that is, when the problem is highly oscillatory.

3 The new family of methods.

In what follows, we will restrict our attention to the second order scalar autonomous initial value problem

$$y''(x) = f(y(x)), \quad y(x_0) = y_0, \quad y'(x_0) = z_0, \quad f : \mathbb{R} \rightarrow \mathbb{R},$$

that is

$$\begin{aligned} y'(x) &= z(x), & y(x_0) &= y_0, \\ z'(x) &= f(y(x)), & z(x_0) &= z_0. \end{aligned}$$

For this problem we will consider the family of two-stage methods given by

$$\begin{aligned} y_{n+1} &= y_n + h (P_1(s) z_n + P_2(s) k_1), \\ z_{n+1} &= Q_1(s) z_n + Q_2(s) k_1, \end{aligned} \tag{5}$$

where functions P_1 , P_2 , Q_1 and Q_2 can be arbitrarily chosen. The stages and the term s are given by

$$\begin{aligned} k_1 &= hf(y_n + hc_1 z_n), \\ k_2 &= hf(y_n + h(c_2 z_n + d_2 k_1)), \\ s &= \frac{k_2 - k_1}{(c_2 - c_1)z_n + d_2 k_1}. \end{aligned} \tag{6}$$

For example, we get the formula of our first example taking the functions

$$\begin{aligned} P_1(s) &= \frac{\text{sen } \sqrt{-s}}{\sqrt{-s}} + \frac{3 - \sqrt{3}}{6} (1 - \cos \sqrt{-s}), \\ P_2(s) &= \frac{\cos \sqrt{-s} - 1}{s}, \\ Q_1(s) &= \cos \sqrt{-s} + \frac{3 - \sqrt{3}}{6} \sqrt{-s} \text{sen } \sqrt{-s}, \\ Q_2(s) &= \frac{\text{sen } \sqrt{-s}}{\sqrt{-s}}, \end{aligned}$$

together with the values of the parameters c_1 , c_2 and d_2 considered in (3).

Now we will study the order conditions for the family of two-stage methods we are considering.

4 Order conditions of the two-stage methods.

We begin considering two-stage methods of the preceding family in which functions P_1 , P_2 , Q_1 and Q_2 are given polynomials, that is

$$\begin{aligned} P_1(s) &= \sum_{i=0}^{p_1} p_{1i} s^i, & P_2(s) &= \sum_{i=0}^{p_2} p_{2i} s^i, \\ Q_1(s) &= \sum_{i=0}^{q_1} q_{1i} s^i, & Q_2(s) &= \sum_{i=0}^{q_2} q_{2i} s^i. \end{aligned} \quad (7)$$

We will define consistency of order q in the same way as is usual with other one-step methods like the Runge-Kutta-Nyström formulae (see for example [6], p. 284).

Definition 1 *Method is said to be consistent (with the special second order problem) of order q , if q is the largest integer such that*

$$y(x_0 + h) - y_1 = O(h^{q+1}), \quad y'(x_0 + h) - z_1 = O(h^{q+1}),$$

It is easily seen when looking for formulas of order four, that it suffices to take $p_1 = p_2 = q_2 = 1$ and $q_1 = 2$ in (7). This follows from the fact that $k_1 = O(h)$ and $s = O(h^2)$, and so all the other parameters appear only when higher order conditions are considered.

Any two-stage method of polynomial type must satisfy the following order

conditions in order to be of order four

$$\begin{aligned}
p_{10} &= 1 & q_{10} &= 1 \\
p_{20} &= 1/2 & q_{20} &= 1 \\
p_{11} + c_1 p_{20} &= 1/6 & q_{11} + c_1 q_{20} &= 1/2 \\
(c_1 + c_2) p_{11} + c_1^2 p_{20} &= 1/12 & (c_1 + c_2) q_{11} + c_1^2 q_{20} &= 1/3 \\
p_{21} &= 1/24 & q_{21} &= 1/6 \\
& & (c_1^2 + c_1 c_2 + c_2^2) q_{11} + c_1^3 q_{20} &= 1/4 \\
& & (c_1 + c_2) q_{21} + d_2 q_{11} &= 1/4 \\
& & q_{12} + c_1 q_{21} &= 1/24
\end{aligned}$$

where we obtain the first five conditions from the approximation to the solution y and all the other conditions from the approximation to $z = y'$. The solution to the above system is

$$\begin{aligned}
c_1 &= \frac{3 \mp \sqrt{3}}{6}, \quad c_2 = \frac{3 \pm \sqrt{3}}{6}, \quad d_2 = \frac{\pm \sqrt{3}}{6}, & (8) \\
p_{10} &= 1, \quad p_{20} = \frac{1}{2}, \quad p_{11} = \frac{-1 \pm \sqrt{3}}{12}, \quad p_{21} = \frac{1}{24}, \\
q_{10} &= 1, \quad q_{20} = 1, \quad q_{11} = \frac{\pm \sqrt{3}}{6}, \quad q_{21} = \frac{1}{6}, \quad q_{12} = \frac{-3 \pm 2\sqrt{3}}{72}.
\end{aligned}$$

It is also possible to satisfy some of the order conditions for order five (but not all). In fact, in order to obtain the order conditions that a method must satisfy in order to be of order five, all we need is to take now the values $p_2 = 1$ and $p_1 = q_1 = q_2 = 2$ in (7) and then to add to the preceding conditions for order four the following

$$(c_1^2 + c_1 c_2 + c_2^2) p_{11} + c_1^3 p_{20} = 1/20, \quad (9)$$

$$(c_1 + c_2) p_{21} + d_2 p_{11} = 1/20, \quad (10)$$

$$p_{12} + c_1 p_{21} = 1/120, \quad (11)$$

$$(c_1^3 + c_1^2 c_2 + c_1 c_2^2 + c_2^3) q_{11} + c_1^4 q_{20} = 1/5, \quad (12)$$

$$(c_1^2 + c_1 c_2 + c_2^2) q_{21} + (c_1 + 2c_2) d_2 q_{11} = 3/10, \quad (13)$$

$$2(c_1 + c_2) q_{12} + c_1(2c_1 + c_2) q_{21} + c_1 d_2 q_{11} = 1/12, \quad (14)$$

$$d_2 q_{21} = 1/20, \quad (15)$$

$$q_{22} = 1/120, \quad (16)$$

where the first three conditions arise from the approximation to y and the other five from the approximation to $z = y'$.

From the values (8) that we must take to have order four, we can see that six of the order conditions (9–16) cannot be satisfied. Therefore it is not possible to obtain fifth order formulas from the family of two-stage methods we are considering. However, we can minimize the principal part of the local truncation error by satisfying the remaining two order conditions (11) and (16). All we need for that is to take the values

$$p_{12} = \frac{-9 \pm 5\sqrt{3}}{720}, \quad q_{22} = \frac{1}{120}, \quad (17)$$

together with those given in (8) to attain order four.

From the order conditions for the two-stage methods of polynomial type and the values of the parameters that we must take in order to obtain formulas of order four, now it is easy to obtain the order conditions for more general two-stage methods of the family considered. All we need is to consider the Taylor's expansions in terms of s of the functions P_1 , P_2 , Q_1 and Q_2 corresponding to the general two-stage method and then compare with the associated expansions of a method of polynomial type with the same number of stages (taking the same k_1 , k_2 and s in both methods). We will illustrate this by obtaining the two-stage formula of order four given as our first example, which obviously is not of polynomial type.

Remember that this method was given by (1-3), that is, we have

$$\begin{aligned} y_{n+1} &= y_n + h (P_1(s) z_n + P_2(s) k_1), \\ z_{n+1} &= Q_1(s) z_n + Q_2(s) k_1 \end{aligned} \quad (18)$$

where the functions must be taken as follows

$$\begin{aligned} P_1(s) &= \frac{\text{sen } \sqrt{-s}}{\sqrt{-s}} + \frac{3 - \sqrt{3}}{6} (1 - \cos \sqrt{-s}), \\ P_2(s) &= \frac{\cos \sqrt{-s} - 1}{s}, \\ Q_1(s) &= \cos \sqrt{-s} + \frac{3 - \sqrt{3}}{6} \sqrt{-s} \text{sen } \sqrt{-s}, \\ Q_2(s) &= \frac{\text{sen } \sqrt{-s}}{\sqrt{-s}}. \end{aligned} \quad (19)$$

The stages k_1 , k_2 and the term s are given as for the two-stage fourth order methods of polynomial type. Note that parameters c_1 , c_2 and d_2 are those given in (8) taking the upper sign. The expansions in powers of s for the functions P_1 , P_2 , Q_1 and Q_2 (redefined if necessary by continuity when $s = 0$) are given by

$$\begin{aligned}
 P_1(s) &= 1 + \frac{-1 + \sqrt{3}}{12} s + \frac{-9 + 5\sqrt{3}}{720} s^2 + O(s^3), \\
 P_2(s) &= \frac{1}{2} + \frac{1}{24} s + \frac{1}{720} s^2 + O(s^3), \\
 Q_1(s) &= 1 + \frac{\sqrt{3}}{6} s + \frac{-3 + 2\sqrt{3}}{72} s^2 + O(s^3), \\
 Q_2(s) &= 1 + \frac{1}{6} s + \frac{1}{120} s^2 + O(s^3),
 \end{aligned} \tag{20}$$

and it is easily seen that this method is of order four. Moreover, it is not difficult to show that for this formula the principal part of the local truncation error is minimized (it suffices to compare the parameters given in (20) with those obtained in (8) and (17) for methods of polynomial type).

5 A two-stage method for oscillatory problems.

During the last years many different methods have been developed for the numerical integration of oscillatory problems. Between many others we have for example the formulas considered in [7], [8], [13], [14], [15], [10] and [11].

Now we will see how to obtain the method (1-3) we have considered to introduce this work, that is, the two stage method given by formulas such as (5-6) that performs well when applied to the numerical integration of highly oscillatory problems.

We begin considering the test equation given by

$$y'' = -\alpha y, \quad y(x_0) = y_0, \quad y'(x_0) = z_0, \tag{21}$$

with $\alpha > 0$. This problem has a well know solution that is given by

$$\begin{pmatrix} y(x) \\ z(x) \end{pmatrix} = \begin{pmatrix} \cos(\sqrt{\alpha}(x-x_0)) & \frac{\text{sen}(\sqrt{\alpha}(x-x_0))}{\sqrt{\alpha}} \\ -\sqrt{\alpha} \text{sen}(\sqrt{\alpha}(x-x_0)) & \cos(\sqrt{\alpha}(x-x_0)) \end{pmatrix} \begin{pmatrix} y_0 \\ z_0 \end{pmatrix} \quad (22)$$

where with z we denote y' . In what follows we will assume (without losing generality) that $x_0 = 0$. Note that when we take nonnegative values for α with $\alpha \gg 1$ the solution presents fast oscillations and therefore it is usually difficult to integrate numerically this problem without taking very small steps sizes.

When we apply a two stage formula of the preceding family of methods given by (5–6) to the test equation we get for the stages

$$\begin{aligned} k_1 &= -h\alpha(y_n + h c_1 z_n), \\ k_2 &= -h\alpha\left((1 - h^2\alpha d_2)y_n + h(c_2 - h^2\alpha d_2 c_1)z_n\right), \end{aligned}$$

and so term s takes the form

$$s = -h^2\alpha.$$

Therefore, formula (5) when applied to the test equation is

$$\begin{pmatrix} y_{n+1} \\ z_{n+1} \end{pmatrix} = \begin{pmatrix} 1 - h^2\alpha P_2(-h^2\alpha) & h(P_1(-h^2\alpha) - h^2\alpha c_1 P_2(-h^2\alpha)) \\ -h\alpha Q_2(-h^2\alpha) & Q_1(-h^2\alpha) - h^2\alpha c_1 Q_2(-h^2\alpha) \end{pmatrix} \begin{pmatrix} y_n \\ z_n \end{pmatrix} \quad (23)$$

From the exact solution (22) (with $x_0 = 0$) it follows that

$$\begin{aligned} \begin{pmatrix} y(x+h) \\ z(x+h) \end{pmatrix} &= \begin{pmatrix} \cos(\sqrt{\alpha}(x+h)) & \frac{\text{sen}(\sqrt{\alpha}(x+h))}{\sqrt{\alpha}} \\ -\sqrt{\alpha} \text{sen}(\sqrt{\alpha}(x+h)) & \cos(\sqrt{\alpha}(x+h)) \end{pmatrix} \begin{pmatrix} y_0 \\ z_0 \end{pmatrix} \\ &= \begin{pmatrix} \cos(\sqrt{\alpha}h) & \frac{\text{sen}(\sqrt{\alpha}h)}{\sqrt{\alpha}} \\ -\sqrt{\alpha} \text{sen}(\sqrt{\alpha}h) & \cos(\sqrt{\alpha}h) \end{pmatrix} \begin{pmatrix} y(x) \\ z(x) \end{pmatrix}, \end{aligned} \quad (24)$$

holds.

When integrating with fixed step size h problem (21) with any of the methods we are considering, y_n and z_n in (23) must approximate the quantities $y(nh)$ and $z(nh)$ of (24) respectively.

If we want to obtain numerical solutions for this problem, being exact except for round-off errors, all we need is to take the matrix in (23) equal to the second matrix in (24). In this way we get that functions P_i and Q_i must satisfy

$$\begin{aligned} P_1(-h^2\alpha) &= \frac{\text{sen}(\sqrt{\alpha}h)}{\sqrt{\alpha}h} + c_1 \left(1 - \cos(\sqrt{\alpha}h)\right), \\ P_2(-h^2\alpha) &= \frac{1 - \cos(\sqrt{\alpha}h)}{h^2\alpha}, \\ Q_1(-h^2\alpha) &= \cos(\sqrt{\alpha}h) + c_1\sqrt{\alpha}h \text{sen}(\sqrt{\alpha}h), \\ Q_2(-h^2\alpha) &= \frac{\text{sen}(\sqrt{\alpha}h)}{\sqrt{\alpha}h}. \end{aligned}$$

Finally, from relation $s = -h^2\alpha$ it is easily seen that the first formula considered in this work integrates exactly oscillatory problems given by $y'' = -\alpha y + \beta$ with $\alpha > 0$ and $\beta \in \mathbb{R}$. Also, as we have seen before, for this method the parameters c_1 , c_2 and d_2 are given as in (3) and so the method is of order four when applied to problem (1) and the principal part of the local truncation error is minimized.

Note that when applying the method to problems for which $s \geq 0$ in some step, then the resulting formula appears to be not well defined (if $s > 0$ then $\sqrt{-s}$ is not defined in \mathbb{R} and if $s = 0$ then some indeterminacies emerge). This situation, that obviously never occurs when only methods of polynomial type are considered, can be easily solved by taking into account that when $s > 0$ we can take $\sqrt{-s} = i\sqrt{s}$ and then, by using the following well known properties

$$\text{ch}(z) = \cos(iz), \quad \text{sh}(z) = -i \text{sen}(iz), \quad z \in \mathbb{C},$$

functions P_i and Q_i can be put in the form

$$\begin{aligned} P_1(s) &= \frac{\text{sh}\sqrt{s}}{\sqrt{s}} + \frac{3 - \sqrt{3}}{6} \left(1 - \text{ch}\sqrt{s}\right), \\ P_2(s) &= \frac{\text{ch}\sqrt{s} - 1}{s}, \\ Q_1(s) &= \text{ch}\sqrt{s} - \frac{3 - \sqrt{3}}{6} \sqrt{s} \text{sh}\sqrt{s}, \end{aligned}$$

$$Q_2(s) = \frac{\text{sh } \sqrt{s}}{\sqrt{s}}, \quad (25)$$

when $s > 0$. When $s = 0$ it suffices to take

$$P_1(s) = 1, \quad P_2(s) = \frac{1}{2}, \quad Q_1(s) = 1, \quad Q_2(s) = 1,$$

as can be seen by solving the indeterminacies.

From the preceding observations it is now clear that our first method integrates exactly (except for round-off errors) any problem given by $y'' = -\alpha y + \beta$ with $\alpha, \beta \in \mathbb{R}$ (note that now $\alpha > 0$ is not assumed).

6 Numerical experiments.

In order to show the behaviour of the two stage methods of order four that we have obtained, we will consider the simple problem given in (4) taking different values for the parameter α . We will integrate this problem, taking various fixed step sizes, with methods:

- (i) The three stage Runge-Kutta-Nyström method of order four given in [6], pp. 285, and marked RKN43.
- (ii) The fourth order two stage method of polynomial type that we obtain from (5), (6) and (7) taking the upper sign in (8) and the remaining parameters equal to zero. This method is marked MSO42.
- (iii) The fourth order two stage method of polynomial type we get from (5), (6) and (7) taking the upper sign in (8) and (17). This method, whose principal part of the local truncation error is minimized, is marked MSO42M.
- (iv) The fourth order two stage method been exact for problems given by $y'' = -\alpha y + \beta$ with $\alpha, \beta \in \mathbb{R}$. This method is marked MSO42T.

The exact solution to problem (4) is not available and so we will consider the error measured with respect to a reference numerical solution carefully calculated with the Gear single-step method (using "bstoer" option, that is, a Burlirsch-Stoer rational extrapolation method) implemented in MAPLEV. The estimated errors are required to be less than 10^{-15} in each component (allowing very small step sizes). We also measured the error with respect to the first integral $(\alpha y^2 + y'^2)/2 - \varepsilon y^4/4$ in some of the numerical experiments.

Figures 1 and 2 show the errors for the solution and its derivative obtained

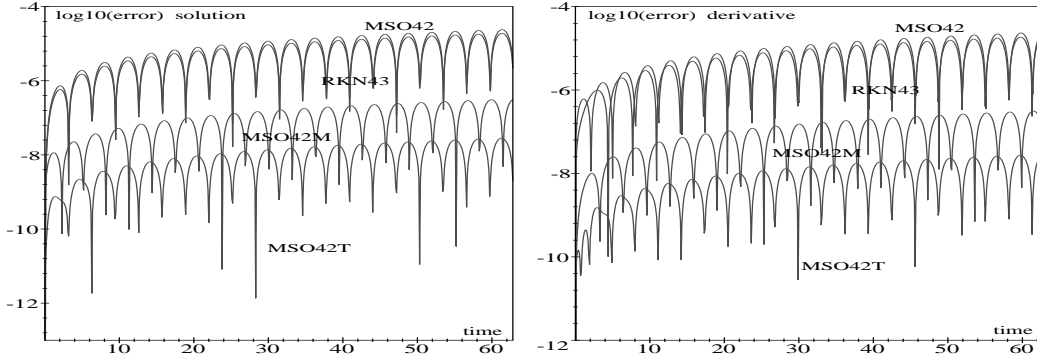


Fig. 1. Error in y for $y'' = -y + 10^{-3}y^3$, Fig. 2. Error in y' for $y'' = -y + 10^{-3}y^3$, $y(0)=1$, $y'(0)=0$, $h=0.1$, $t \in [0, 20\pi]$.

when above methods are applied to problem

$$y'' = -\alpha y + \varepsilon y^3, \quad y(0) = 1, \quad y'(0) = 0,$$

taking the values $\alpha = 1$ and $\varepsilon = 10^{-3}$, and integrating with fixed step size $h = 0.1$ over the interval $[0, 20\pi]$ (that is 10 revolutions).

Figure 3 shows the numerical results (taking the same values as in figures 1 and 2) for the errors measured with respect to the first integral.

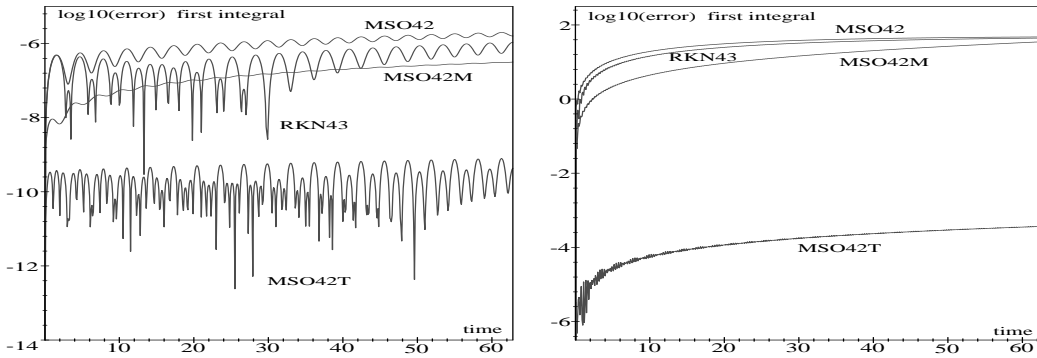


Fig. 3. Error for $y'' = -y + 10^{-3}y^3$, $y(0)=1$, Fig. 4. Error for $y'' = -100y + 10^{-3}y^3$, $y(0)=1$, $y'(0)=0$, $h=0.1$, $t \in [0, 20\pi]$.

We can observe in the preceding figures that the errors are smaller for method marked MSO42T. Formulas marked MSO42 and MSO42M perform more or less as the Nyström method marked RKN43, but note that both need one less evaluation per step.

We repeat the preceding numerical experiment but now taking $\alpha = 100$ (the other values as before) so that the problem becomes highly oscillatory. We show the errors (measured with respect to the first integral) in figure 4. It can be observed in this figure that the only formula that gives a satisfactory

approximation is the one marked MSO42T, that is, the only one method we have developed in order to perform well when oscillatory problems are considered.

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