

A symplectic explicit trigonometrically-fitted Runge-Kutta-Nyström method for the numerical solution of periodic problems

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Abstract

In this paper, symplectic third-order three-stage explicit trigonometrically-fitted Runge-Kutta-Nyström (RKN) method for the numerical solution of second order initial value problems with periodic solutions is derived. The numerical results show the accuracy of the new method in comparison with other existing symplectic and non-symplectic RKN methods.

INTRODUCTION

In the last two decades, methods for the numerical solution of the initial value problems

$$\begin{aligned} y'' &= f(x, y), & x \in [x_0, X], \\ y(x_0) &= y_0, & y'(x_0) = y'_0, \end{aligned} \quad (1)$$

whose solution has a pronounced periodic/oscillatory behavior has attracted the interest of many researchers. Such problems occur in several fields of applied sciences such as: molecular dynamics, celestial mechanics, theoretical physics, physical chemistry, nuclear physics and electronics. Van de Vyver in [2,3,4] proposed a symplectic exponentially fitted modified Runge-Kutta-Nyström method for the numerical integration of orbital problems, a fourth-order symplectic exponentially fitted integrator and a symplectic Runge-Kutta-Nyström method with minimal phase-lag. Tocino and Vigo-Aguiar in [5] proposed symplectic conditions for exponential fitting Runge-Kutta-Nyström methods. Recently, Kalogiratou et al in [6] proposed a fourth order modified trigonometrically fitted symplectic Runge-Kutta-Nyström method. More recently, Franco and Gomez in [7] proposed symplectic explicit methods of Runge-Kutta-Nyström type for solving perturbed oscillators. Symplectic methods are widely used for solving Hamiltonian systems.

Hamiltonian systems are first order ODEs that can be expressed as:

$$\frac{dy}{dt} = -\frac{\partial H}{\partial x}, \quad \frac{dx}{dt} = \frac{\partial H}{\partial y}$$

where $x, y \in \mathbb{R}^d$ and H is a twice continuously differentiable function $H: U \rightarrow \mathbb{R}^{2d}$ ($U \subset \mathbb{R}^{2d}$ is an open set). Symplecticity is a behavioral property of Hamiltonian systems. Therefore it is by default necessary to search for a numerical methods that share this property. Much emphasis has been given to symplectic integrators for the numerical solution of Hamiltonian systems (see Hairer et al., 2002). Although, it is at most certain that the local error of a non-symplectic method is smaller than that of the symplectic method, the error generated during the integration process is slower for the symplectic method. Thus, for a long-time integration of Hamiltonian systems the symplectic method will

be more accurate than the non-symplectic method. A simple example to show how a symplectic method is propagated is by the use of an undamped harmonic oscillator. In this study, our main attention is on the systems of second order ODEs (1); which is a generalized representation of periodic problems; In which the first derivative does not appear explicitly. After changing the ODE (1) in to an equivalent system of first order ODEs, we get a Hamiltonian system. Beside the symplecticity, one can take in to account that the solutions of the ODE (1) have a periodic behavior. In that case trigonometric fitting is a suitable choice. Motivated by the work of Simos in [8], we develop a symplectic third-order three-stage and third-order four-stage explicit trigonometrically-fitted RKN methods. The remaining part of this paper is designed as follows: In section 2 we give the basic theory of an explicit Runge-Kutta-Nyström method, Hamiltonian system, construction of Hamiltonian system and definition of a symplectic RKN method. Section 3 deals with the derivation of the proposed method. In section 4 we analyze the algebraic order of the new method from its local truncation error. In section 5 we present the numerical results and the last section deals with the conclusion.

BASIC THEORY

The general form of an explicit m -stage RKN method is given by:

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{i=1}^m b_i f(x_n + c_i h, Y_i), \quad (2)$$

$$y'_{n+1} = y'_n + h \sum_{i=1}^m d_i f(x_n + c_i h, Y_i), \quad (3)$$

$$Y_i = y_n + c_i h y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, Y_j). \quad (4)$$

Or in Butcher Tableau as:

c	A
b	
d	

where a_{ij} , b_j , d_j and c_j are the RKN parameters which are assumed to be real and m is the number of stages of the method. Introducing the m -dimensional vectors c, b, d and $m \times m$ matrix A , where $c = [c_1, c_2, \dots, c_m]^T$, $b = [b_1, b_2, \dots, b_m]^T$, $d = [d_1, d_2, \dots, d_m]^T$, $A = [a_{ij}]$, respectively.

Hamiltonian Systems

Hamiltonian systems are linear or nonlinear systems with particular symmetry that allows the stability of equilibrium points to be found and the solutions curves to be drawn even though actual solutions are not obtained. For these systems, the derivatives $\frac{dx}{dt}$ and $\frac{dy}{dt}$ are partial derivatives of a function called Hamiltonian function $(H(x, y))$.

$$\frac{dx}{dt} = \frac{\partial H}{\partial y}$$

$$\frac{dy}{dt} = -\frac{\partial H}{\partial x}$$

Now, in terms of the variables of the systems we have: $\frac{\partial}{\partial x} \frac{dx}{dt} = -\frac{\partial}{\partial y} \frac{dy}{dt}$. Which enable us to write the system as:

$$\frac{dx}{dt} = f(x, y),$$

$$\frac{dy}{dt} = g(x, y).$$

Therefore, a system is Hamiltonian if: $\frac{\partial f}{\partial x} = -\frac{\partial g}{\partial y}$. In other words, a system that is Hamiltonian can be identified by this property. For example, the undamped harmonic oscillator $y'' = -100y$ is a linear Hamiltonian system. Changing this in to an equivalent system of first order ODEs, we have:

$$x' = y = f(x, y),$$

$$y' = -100x = g(x, y).$$

From above, we can see that: $\frac{\partial f}{\partial x} = \frac{dy}{dx} = 0$ and $\frac{\partial g}{\partial y} = 0$

Therefore, $\frac{\partial f}{\partial x} = -\frac{\partial g}{\partial y}$ implying that the undamped harmonic oscillator is a Hamiltonian system.

Constructing Hamiltonian Systems

The integral $\int \frac{\partial H}{\partial y} dy$ allows the Hamiltonian function to be determined up to a function that depends only on x : $H(x, y) = \int \frac{\partial H}{\partial y} dy + \Phi(x) = \int f(x, y) dy + \Phi(x)$, using the other system variable

$$\frac{\partial H}{\partial x} = -g(x, y),$$

$$= \frac{\partial}{\partial x} \int f(x, y) dy + \frac{d}{dx} \Phi(x).$$

Rearranging we have:

$$\frac{d}{dx} \Phi(x) = -g(x, y) - \frac{\partial}{\partial x} \int f(x, y) dy.$$

Integrating $f(x, y)$ with respect to x , we have:

$$H(x, y) = \int f(x, y) dy + \Phi(x)$$

Integrating both side with respect to x of equation (6), we have:

$$\Phi(x) = \int \frac{d}{dx} \Phi(x) dx + C$$

Setting $C = 0$ and substituting equation (8) in (7), we have the Hamiltonian.

Definition 1. A Runge-Kutta-Nyström method (2) - (4) is said to be symplectic if it satisfies these two conditions:

$$b_i = d_i(1 - c_i), i = 1, 2, \dots, m, \tag{9}$$

$$a_{ij} = d_j(c_i - c_j), i, j = 1, 2, \dots, m. \tag{10}$$

Or equivalently,

$$\det \begin{bmatrix} \frac{\partial y_{n+1}}{\partial y_n} & \frac{\partial y_{n+1}}{\partial y'_n} \\ \frac{\partial y'_{n+1}}{\partial y_n} & \frac{\partial y'_{n+1}}{\partial y'_n} \end{bmatrix} = 1.$$

Definition 2. A Runge-Kutta-Nyström method (2)-(4) is said to be trigonometrically-fitted if it integrates exactly the function e^{iwx} and e^{-iwx} or equivalently $\sin(wx)$ and $\cos(wx)$ with $w > 0$ the principal frequency of the problem when applied to the test equation $y'' = -w^2y$; Leading to a system of equations as derived in the next section.

CONSTRUCTION OF THE NEW METHOD

In this section, we will derive a three-stage third order symplectic explicit trigonometrically-fitted RKN methods. In this study, a third-order three-stage with phase-lag order six and a third-order four-stage with phase-lag order six as derived by Mohamad in [10] will be considered. The coefficients of the third-order three-stage method are given in Table 1 and that of the third-order four-stage method are given in Table 2 below:

Table 1: The SRKN3(3,6) Method [10]

0.630847693	0.164217030		
0.536704894	0.139710559	-0.103005664	
	0.260311692	0.4039053382	-0.164217030
	0.260311692	1.094142798	-0.354454490

Table 2: The SRKN4(3,6) Method [10]

0				
$\frac{1}{4}$	0.01735693			
$\frac{3}{4}$	0.0520708	0.2201621		
0.6015339	0.04176314	0.1547889	-0.0950181	
	0.06942774	0.3302431	0.15999974	-0.0596706
	0.06942774	0.4403242	0.63999897	-0.1497509

Applying an explicit Runge-Kutta-Nyström method (2) - (4) for $m = 3$ to the test equation $y'' = -w^2y$, we obtained:

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{i=1}^3 b_i (-w^2 Y_i),$$

and

$$y'_{n+1} = y'_n + h \sum_{i=1}^3 d_i (-w^2 Y_i).$$

where

$$Y_i = y_n + c_i h y'_n + h^2 \sum_{j=1}^3 a_{ij} (-w^2 Y_j). \quad (13)$$

Let $y_n = e^{Iwx}$, $y'_n = Iwe^{Iwx}$, $y_{n+1} = e^{Iw(x+h)}$ and $y'_{n+1} = Iwe^{Iw(x+h)}$ and substituting in the equations (11) - (13) and by using $e^{Iv} = \cos(v) + I \sin(v)$ and comparing the real and imaginary part, we get the following system of equations:

$$\cos(v) = 1 - v^2 \sum_{i=1}^3 b_i (1 - v^2 \sum_{j=1}^2 a_{ij} Y_j e^{-Iwx}), \quad (14)$$

$$\sin(v) = v - v^2 \sum_{i=1}^3 b_i c_i v, \quad (15)$$

$$\sin(v) = v \sum_{i=1}^3 d_i (1 - v^2 \sum_{j=1}^2 a_{ij} Y_j e^{-Iwx}), \quad (16)$$

$$\cos(v) = 1 - v^2 \sum_{i=1}^3 d_i c_i. \quad (17)$$

where $v = wh$.

Solving (14)-(17) using the coefficients of the method in TABLE 1 for b_2, b_3, d_2, c_3 , we obtain the Taylor series expansion of the solution as given in (18)

$$\begin{aligned} b_2 &= 0.4039053385 + 0.01030056827 v^2 \\ &\quad - 0.01134471884 v^4 \\ &\quad - 0.006820875217 v^6 \\ &\quad - 0.002769825468 v^8 \\ &\quad - 0.0009870934773 v^{10} \\ &\quad - 0.0003300631147 v^{12} + \dots, \\ b_3 &= -0.1642170317 + 0.008333332625 v^2 \\ &\quad + 0.01195323338 v^4 \\ &\quad + 0.005512780698 v^6 \\ &\quad + 0.002054535630 v^8 \\ &\quad + 0.0007009006713 v^{10} \\ &\quad + 0.0002284451153 v^{12} \\ &\quad + 0.00007253906197 v^{14} + \dots, \\ d_2 &= 1.094142798 - 0.0000000001000000000 v^2 \\ &\quad + 0.002337634796 v^4 \\ &\quad + 0.0001854667464 v^6 \\ &\quad + 0.00003321253029 v^8 \\ &\quad + 0.000005429010995 v^{10} \\ &\quad + 0.0000008916966550 v^{12} \\ &\quad + 0.0000001464310122 v^{14} \\ &\quad + 0.00000002404646882 v^{16} + \dots, \\ c_3 &= 0.5367048946 + 0.05257064094 v^2 \\ &\quad + 0.0002420695272 v^4 \\ &\quad + 0.0004000594164 v^6 \\ &\quad + 0.00005833322898 v^8 \\ &\quad + 0.000009668284179 v^{10} \\ &\quad + 0.000001586983162 v^{12} \\ &\quad + 0.0000002606137506 v^{14} + \dots \end{aligned} \quad (18)$$

This lead to the new method denoted as SETFRKN3(3,6).

ALGEBRAIC ORDER AND ERROR ANALYSIS

In this section, we perform local truncation error analysis, based on the Taylor series expansion of the actual solution $y(x_n + h)$, the first derivative of the actual solution $y'(x_n + h)$, the approximate solution y_{n+1} and the first derivative of the approximate solution y'_{n+1} . The local truncation error (LTE) of y and its first derivative y' is given in (19).

$$\begin{aligned} LTE &= y_{n+1} - y(x_n + h), \\ LTE_{der} &= y'_{n+1} - y'(x_n + h). \end{aligned} \quad (19)$$

The principal terms of the LTE for y and y' of the new method SETFRKN3(3,6) is given in (20), where it is shown that the order of the new method is four.

$$\begin{aligned} [!ht] \\ PLTE &= -h^4 (0.01552663125186008177 f_{xx} \\ &\quad + 0.030105326250372016357 y' f_{xy} \\ &\quad + 0.015052663125186008177 (y')^2 f_{yy} \\ &\quad + 0.01863389980879612944 f_y y'' \\ &\quad + 0.018633900895 w^2) + O(h^5), \\ PLTE_{der} &= \frac{h^4}{24} (f_{xxx} + 3y' f_{yxx} + 3y'' f_{xy} + 3(y')^2 f_{xyy} \\ &\quad + 3y' f_{yy} y'' + (y')^3 f_{yyy} + f_y f_x \\ &\quad + (f_y)^2 y') + O(h^5). \end{aligned} \quad (20)$$

PROBLEMS TESTED AND NUMERICAL RESULTS

In this section, we will apply the new method to some second-order ordinary differential equation problems. The following methods are used for the numerical comparisons.

- SETFRKN3(3,6): The new three-stage third order symplectic explicit trigonometrically-fitted RKN method derived in this paper,
- SRKN3(3,6): The three-stage third order symplectic explicit RKN method with phase-lag order six derived by Mohamad in [10],
- RKN4G: The fourth-order three-stage RKN method derived by Garcia in [1], and
- RKN3(3,6, ∞): The three-stage third order explicit RKN method with phase-lag order six and zero dissipative derived by Senu in [9].

Problem 1. (Harmonic Oscillator) Anastassi and Kosti in [11]

$$y'' = -100y, y(0) = 1, y'(0) = 2,$$

The exact solution is

$$y(x) = -\frac{1}{5} \sin(10x) + \cos(10x).$$

Problem 2. (Almost Periodic Problem) Mohamad in [10]

$$y_1'' = -y_1 + 0.001 \cos(x), y_1(0) = 1, y_1'(0) = 0,$$

$$y_2'' = -y_2 + 0.001 \sin(x), y_2(0) = 0, y_2'(0) = 0.9995,$$

The exact solution is

$$y_1(x) = \cos(x) + 0.0005 x \cos(x),$$

$$y_2(x) = \sin(x) - 0.0005 x \sin(x).$$

Problem 3. Anastassi and Kosti in [11]

$$y'' = -v^2 y(x) + (v^2 - 1) \sin(x), \quad y(0) = 1, \quad y'(0) = v + 1, \quad x \geq 0, \quad \text{where } v \gg 1,$$

The exact solution is

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

Problem 4. Senu in [9]

$$y'' = -y + x, \quad y(0) = 1, \quad y'(0) = 2,$$

The exact solution is

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

The accuracy strategy used is finding \log_{10} of the maximum global error,

$$\text{MAXERR} = \log_{10} \max \|y(x_n) - y_n\|,$$

(21)

where $x_n = x_0 + nh$, $n = 1, 2, 3, \dots, (T - x_0)/h$. In this paper, we denote T as the interval used for the integration.

The numerical results are shown in Tables 3-6.

Table 3: Numerical results for problem 1

h	Methods	T = 1000	T = 5000	T = 10000
0.025	SRKN3(3,6)	2.909168(-4)	2.909168(-4)	3.3.289169(-4)
	SETFRKN3(3,6)	1.803259(-6)	9.021893(-6)	1.739035(-5)
	RKN4G	6.205026(-2)	3.052327(-1)	5.935375(-1)
0.05	RKN3(3,6,∞)	2.909152(-4)	2.909152(-4)	3.435898(-4)
	SRKN3(3,6)	2.348434(-3)	1.823382(-2)	3.874725(-2)
	SETFRKN3(3,6)	1.614799(-5)	8.076988(-5)	1.616481(-4)
0.075	RKN4G	8.664679(-1)	1.540438(+0)	1.540438(+0)
	RKN3(3,6,∞)	2.348432(-3)	1.824115(-2)	3.876189(-2)
	SRKN3(3,6)	4.110906(-2)	2.372272(-1)	4.791851(-1)
0.1	SETFRKN3(3,6)	7.870694(-3)	3.874390(-2)	7.608979(-2)
	RKN4G	1.391214(+0)	1.391214(+0)	1.391214(+0)
	RKN3(3,6,∞)	4.111048(-2)	2.372344(-1)	4.791997(-1)
0.1	SRKN3(3,6)	2.752468(-1)	1.339798(+0)	2.020189(+0)
	SETFRKN3(3,6)	4.798225(-1)	9.937901(-1)	1.021369(+0)
	RKN4G	1.279301(+0)	1.279301(+0)	1.279301(+0)
0.1	RKN3(3,6,∞)	2.752481(-1)	1.339805(+0)	2.020196(+0)

Table 4: Numerical results for problem 2

h	Methods	T = 1000	T = 5000	T = 10000
0.025	SRKN3(3,6)	4.549746(-7)	1.674375(-6)	4.578916(-6)
	SETFRKN3(3,6)	1.857857(-7)	1.503431(-6)	4.474197(-6)
	RKN4G	6.268906(-7)	4.866342(-6)	1.613212(-5)
0.05	RKN3(3,6,∞)	3.221998(-7)	7.468672(-7)	1.142362(-6)
	SRKN3(3,6)	2.569510(-6)	5.142489(-6)	1.068136(-5)
	SETFRKN3(3,6)	6.662229(-7)	4.107931(-6)	9.998485(-6)
0.075	RKN4G	1.004116(-5)	7.811003(-5)	2.627705(-4)
	RKN3(3,6,∞)	2.581249(-6)	6.114042(-6)	1.144586(-5)
	SRKN3(3,6)	8.320939(-6)	1.445156(-5)	2.668259(-5)
0.1	SETFRKN3(3,6)	2.134144(-6)	1.142930(-5)	2.484904(-5)
	RKN4G	5.084022(-5)	3.953611(-4)	1.330306(-3)
	RKN3(3,6,∞)	8.703650(-6)	2.051119(-5)	3.877658(-5)
0.1	SRKN3(3,6)	1.953365(-5)	3.263652(-5)	5.745523(-5)
	SETFRKN3(3,6)	5.020719(-6)	2.590202(-5)	5.376943(-5)
	RKN4G	1.606798(-4)	1.249630(-3)	4.205253(-3)
0.1	RKN3(3,6,∞)	2.062338(-5)	4.856175(-5)	9.155271(-5)

Table 5: Numerical results for problem 3

h	Methods	T = 1000	T = 5000	T = 10000
0.025	SRKN3(3,6)	3.020171(-4)	3.020171(-4)	6.655309(-4)
	SETFRKN3(3,6)	2.605118(-6)	1.258396(-5)	2.421778(-5)
	RKN4G	8.609385(-2)	4.233520(-1)	8.230410(-1)
0.05	RKN3(3,6,∞)	3.021801(-4)	3.062383(-4)	6.863074(-4)
	SRKN3(3,6)	4.293087(-3)	2.676248(-2)	5.522888(-2)
	SETFRKN3(3,6)	2.310649(-5)	1.126541(-4)	2.249074(-4)
0.075	RKN4G	1.201341(+0)	1.201341(+0)	1.201341(+0)
	RKN3(3,6,∞)	4.297201(-3)	2.677425(-2)	5.524999(-2)
	SRKN3(3,6)	6.228579(-2)	3.347018(-1)	6.711267(-1)
0.1	SETFRKN3(3,6)	1.089897(-2)	5.375634(-2)	1.055514(-1)
	RKN4G	1.929449(+0)	1.929449(+0)	1.929449(+0)
	RKN3(3,6,∞)	6.229966(-2)	3.347039(-1)	6.711440(-1)
0.1	SRKN3(3,6)	3.960430(-1)	1.879627(+0)	2.824299(+0)
	SETFRKN3(3,6)	6.657655(-1)	1.378237(+0)	1.416410(+0)
	RKN4G	1.773207(+0)	1.773207(+0)	1.773207(+0)
0.1	RKN3(3,6,∞)	3.960249(-1)	1.879651(+0)	2.824317(+0)

Table 6: Numerical results for problem 4

h	Methods	T = 1000	T = 5000	T = 10000
0.025	SRKN3(3,6)	4.647316(-7)	1.277958(-6)	2.228004(-6)
	SETFRKN3(3,6)	2.114488(-7)	1.058883(-6)	2.019522(-6)
	RKN4G	8.611927(-7)	4.310487(-6)	8.524657(-6)
0.05	RKN3(3,6,∞)	2.921239(-7)	3.027080(-7)	3.027080(-7)
	SRKN3(3,6)	2.494562(-6)	3.180916(-6)	4.096439(-6)
	SETFRKN3(3,6)	2.132899(-7)	1.083105(-6)	2.133578(-6)
0.075	RKN4G	1.379246(-5)	6.903953(-5)	1.380617(-4)
	RKN3(3,6,∞)	2.344371(-6)	2.351930(-6)	2.362362(-6)
	SRKN3(3,6)	8.080317(-6)	8.668262(-6)	9.468105(-6)
0.1	SETFRKN3(3,6)	2.165141(-7)	1.073267(-6)	2.168899(-6)
	RKN4G	6.981822(-5)	3.493498(-4)	6.991754(-4)
	RKN3(3,6,∞)	7.939240(-6)	7.939240(-6)	7.939240(-6)
0.1	SRKN3(3,6)	1.900296(-5)	1.948996(-5)	2.013470(-5)
	SETFRKN3(3,6)	2.195048(-7)	1.098892(-6)	2.223069(-6)
	RKN4G	2.207326(-4)	1.104077(-3)	2.209373(-3)
0.1	RKN3(3,6,∞)	1.888495(-5)	1.888495(-5)	1.888495(-5)

We also display the accuracy of these methods graphically in figures 1 to 4.

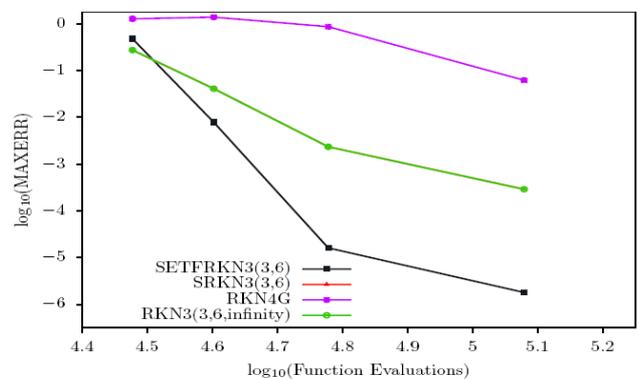


Figure 1. The efficiency curve for Problem 1 with $t_{end} = 1000$ and $h = i(0.025), i = 1, 2, 3, 4$.

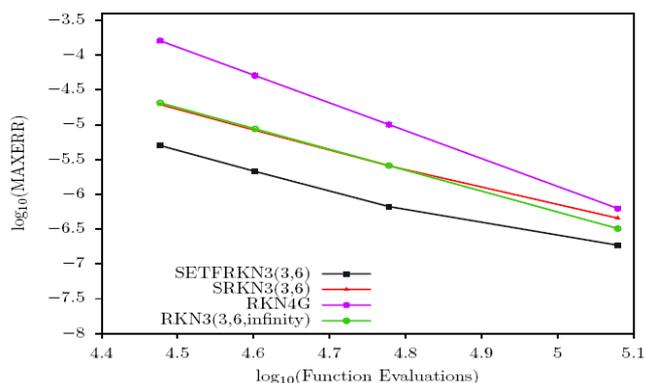


Figure 2. The efficiency curve for Problem 2 with $t_{end} = 1000$ and $h = i(0.025), i = 1,2,3,4$.

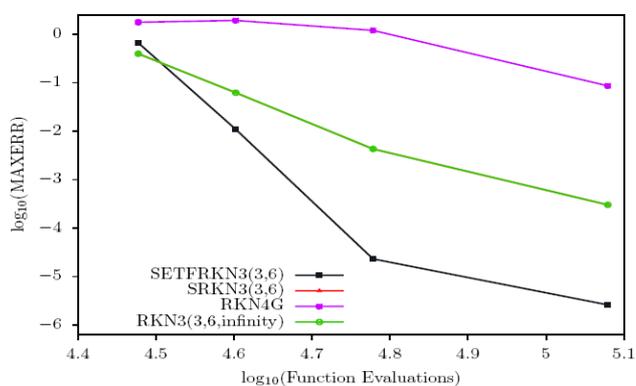


Figure 3. The efficiency curve for Problem 3 with $t_{end} = 1000$ and $h = i(0.025), i = 1,2,3,4$.

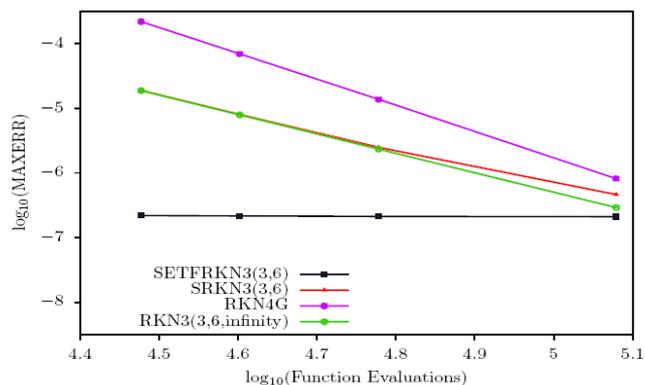


Figure 4. The efficiency curve for Problem 4 with $t_{end} = 1000$ and $h = i(0.025), i = 1,2,3,4$.

CONCLUSION

In this work, we have presented a third order three-stage and a third order four-stage symplectic explicit trigonometrically-fitted RKN methods for the solutions of periodic problems. The numerical results of the new methods are compared with other existing symplectic and non symplectic RKN methods. The global error of the new methods is smaller than the other existing methods. Hence, the new

methods are more accurate and efficient for solving periodic second order ODEs.

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