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Symplectic Runge-Kutta-Nyström Methods with Phase-Lag Oder 8 and Infinity

Z. Kalogiratou[1], *Th. Monovasilis*[2] *and T. E. Simos* [3,4,*]

[1] Department of Informatics and Computer Technology, Technological Educational Institution of Western Macedonia at Kastoria, Kastoria, P.O. Box. 30, 52100 Greece.
[2] Department of International Trade, Technological Educational Institution of Western Macedonia at Kastoria, Kastoria, P.O. Box. 30, 52100 Greece.
[3] Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia.
[4] Laboratory of Computational Sciences, Department of Computer Science and Technology, University of Peloponnese, GR-221 00 Tripolis, Greece.

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Abstract: In this work we consider Symplectic Runge Kutta Nyström methods with five stages. A new fourth algebraic order method with phase-lag order eight is presented. Also the symplectic Runge Kutta Nyström of Calvo and Sanz Serna with five stages and fourth order is modified to produce a phase-fitted method. We apply the new methods on several Hamiltonian systems and on the computation of the eigenvalues of the Schrödinger Equation.

Keywords: . Runge Kutta Nyström methods, Hamiltonian systems, Schrödinger Equation, Phase-lag.

1 Introduction

In this paper we consider systems of second order ODEs of the form

$$y''(x) = f(x,y(x)), \quad x \in [x_0,X], \tag{1}$$
$$y(x_0) = y_0, \quad y'(x_0) = y'_0.$$

Many categories of numerical methods have been developed for the numerical solution of the special problem (1), among them are Runge-Kutta-Nyström (RKN) methods (for more details see [1] - [85] and references therein). The most well known are the methods developed by Dormand and Prince[4], Dormand, El Mikawy and Prince [5][6], these are methods with algebraic order up to eight. Also methods that take into account the nature of the problem have been consider by many authors. There are two categories of such methods with coefficients depending on the problem and with constant coefficients. For the first category a good estimate of the period or of the dominant frequency is needed, such methods are exponentially and trigonometrically fitted methods, phase-fitted and amplification fitted methods. In the second category are methods with minimum phase-lag and P-stable methods and are suitable for every oscillatory problem.

On the other hand research has been performed in the area of numerical integration of Hamiltonian systems with symplectic methods. Let U be an open subset of $\Re^{2d}$, I an open subinterval of $\Re$ then the hamiltonian system of differential equations is given by

$$p' = -\frac{\partial H}{\partial q}(p,q,x), \quad q' = \frac{\partial H}{\partial p}(p,q,x), \tag{2}$$

where $(p,q) \in U$, $x \in I$, the integer d is the number of degrees of freedom and $H(p,q,x)$ be a twice continously differentiable function on $U \times I$. The q variables are generalized coordinates, the p variables are the conjugated generalized momenta and $H(p,q)$ is the total mechanical energy. The solution operator of a Hamiltonian system is a symplectic transformation. A symplectic numerical method preserves the symplectic structure in the phase space when applied to Hamiltonian problems. Symplectic Runge-Kutta-Nyström methods are appropriate methods for the numerical integration of

* Corresponding author e-mail: tsimos.conf@gmail.com

Hamiltonian systems of the special form

$$H(p,q,x)=\frac{1}{2}p^T p+V(q,x). \tag{3}$$

which can be written in the form (1) where y is q. The theory of these methods can be found in the book of Sanz-Serna and Calvo [11].

Some authors in the last decade constructed symplectic RKN methods that are also exponentially/trigonometrically fitted [13,14,16,19]. The phase-lag (or dispersion) property was introduced by Brusa and Nigro [2] and was extended to RK(N) methods by van der Houwen and Sommeijer [15]. This is another type of truncation error the angle between the analytical and the numerical solution. The idea of phase-fitting was introduced by Raptis and Simos [9].

Van de Vyver [17] first constructed a symplectic Runge-Kutta-Nyström method with minimum phase-lag. His method has third algebraic order and sixth phase-lag order. In another work Vyver [18] constructed a four stages fourth algebraic order method with phase-lag order six. In this work we present a five stages fourth order method with phase-lag order eight. Also we modify the five stage fourth order SRKN method of Calvo and Sanz Serna [3] to produce a phase-fitted SPRK method.

In section two the basic theory of RKN methods and the definitions of dispersion and dissipation are given. The new methods are constructed in section 3.Numerical results are presented in section 4 and conclusions in section 5.

2 Symplectic RKN methods

A explicit RKN method is associated with a Butcher tableau

$$\begin{array}{c|cccc} c_1 & & & & \\ c_2 & a_{21} & & & \\ c_3 & a_{31} & a_{32} & & \\ \vdots & \vdots & \vdots & & \\ c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} \\ \hline & \beta_1 & \beta_2 & \cdots & \beta_{s-1} & \beta_s \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array}$$

the RKN method is

$$y_{n+1}=y_n+hy'_n+h^2\sum_{i=1}^{s}\beta_i f_i,$$

$$y'_{n+1}=y'_n+h\sum_{i=1}^{s}b_i f_i, \tag{4}$$

$$f_i=f\left(x_n+c_ih\,,y_n+c_ihy'_n+h^2\sum_{j=1}^{i-1}a_{ij}f_j\right) \tag{5}$$

Suris showed that a RKN method is symplectic when applied to Hamiltonian problems of the form (1) if the coefficients of the method satisfy

$$\beta_i=b_i(1-c_i),\qquad 1\le i\le s, \tag{6}$$

$$b_i(\beta_j-\alpha_{ij})=b_j(\beta_i-\alpha_{ji}),\qquad 1\le i,j\le s. \tag{7}$$

A RKN method that satisfies (6) and (7) is called symplectic RKN method (SRKN).

Condition (6) is a well known simplifying assumption from the standard theory of RKN methods that reduces the number of order conditions. Calvo and Sanz-Serna has shown that condition (7) is also a simplifying assumption.

In the case of explicit RKN methods the coefficients a_{ij} are fully determined by the coefficients b_i and c_i

$$a_{ij}=b_j(c_i-c_j) \tag{8}$$

Phase-lag analysis of numerical methods for second order equations is based on the scalar test equation $q''=-w^2q$, where w is a real constant. For the numerical solution of this equation we can write

$$\begin{pmatrix} q_n \\ h\,p_n \end{pmatrix}=M_n\begin{pmatrix} q_0 \\ h\,p_0 \end{pmatrix},\quad M=\begin{pmatrix} A_s(v^2) & B_s(v^2) \\ C_s(v^2) & D_s(v^2) \end{pmatrix}$$

where $v=wh$. The eigenvalues of the M are called amplification factors of the method and are the roots of the characteristic equation

$$\xi^2-tr(M(v^2))\xi+\det(M(v^2))=0$$

The phase-lag (dispersion) of the method is

$$\phi(v)=v-\arccos\left(\frac{tr(M(v^2))}{2\sqrt{\det(M(v^2))}}\right),$$

and the dissipation (amplification error) is

$$\alpha(v)=1-\sqrt{\det(M(v^2))}.$$

For a SRKN method the determinant of the amplification matrix is zero, so the methods we construct here are zero dissipative.

Then the phase-lag of the method is

$$\phi(v)=v-\arccos\left(\frac{tr(M(v^2))}{2}\right),$$

The trace $tr(M(v^2))$ is a polynomial in v of order $2s$ where s is the number of stages of the SRKN method.

3 Construction of the new methods

We consider the five stage method

$$\begin{array}{c|ccccc} c_1 & & & & & \\ c_2 & b_1(c_2-c_1) & & & & \\ c_3 & b_1(c_3-c_1) & b_2(c_3-c_2) & & & \\ c_4 & b_1(c_4-c_1) & b_2(c_4-c_2) & b_3(c_4-c_3) & & \\ c_5 & b_1(c_5-c_1) & b_2(c_5-c_2) & b_3(c_5-c_3) & b_4(c_5-c_4) & \\ \hline & b_1(1-c_1) & b_2(1-c_2) & b_3(1-c_3) & b_4(1-c_4) & b_5(1-c_5) \\ \hline & b_1 & b_2 & b_3 & b_4 & b_5 \end{array}$$

The order conditions for SRKN methods up to order four are the following

first order

$$b.e = 1,$$

second order

$$b.c.e = \frac{1}{2},$$

third order

$$b.c^2.e = \frac{1}{3}, \quad b.a.e = \frac{1}{6},$$

fourth order

$$b.c^3.e = \frac{1}{4}, \quad b.a.c.e = \frac{1}{24}.$$

The trace of the amplification matrix M can be written as

$$tr(M(v^2)) = 2 - pl_2v^2 + pl_4v^4 - pl_6v^6 + pl_8v^8 - pl_{10}v^{10}$$

where

$$\begin{aligned} pl_2 &= b.c.e + \beta.e, \\ pl_4 &= b.a.c.e + \beta.a.e, \\ pl_6 &= b.a.a.c.e + \beta.a.a.e, \\ pl_8 &= b.a.a.a.c.e + \beta.a.a.a.e, \\ pl_{10} &= b.a.a.a.a.c.e + \beta.a.a.a.a.e \end{aligned}$$

3.1 Method with constant coefficinets

We shall consider the FSAL case by setting $c_1 = 0$ and $c_5 = 1$, then $pl_{10} = 0$. The maximum phase-lag order we can obtain is eigth. We solve the six order conditions together with the phase-lag conditions

$$pl_6 = 2/6!, \quad pl_8 = 2/8!.$$

for c_2,c_3,c_4 and b_i for $i = 1,\ldots,5$.
The following sets of coefficients are obtained

$$\begin{aligned} c_2 &= -0.118848387543557942, \\ c_3 &= 0.539254421314150014, \\ c_4 &= 0.430434893828670465, \\ b_1 &= -0.313702070942374513, \\ b_2 &= 0.273435305462953536, \\ b_3 &= -0.309852240725141981, \\ b_4 &= 1.142156468574106133, \\ b_5 &= 0.207962537630456825 \end{aligned}$$

or

$$\begin{aligned} c_2 &= 0.569565106171329534, \\ c_3 &= 0.460745578685849985, \\ c_4 &= 1.118848387543557940, \\ b_1 &= 0.207962537630456825, \\ b_2 &= 1.142156468574106129, \\ b_3 &= -0.309852240725141980, \\ b_4 &= 0.273435305462953536, \\ b_5 &= -0.313702070942374510 \end{aligned}$$

The leading term of the phase-lag error is

$$\frac{2}{10!}v^{10} = -5.5115\,10^{-7}v^{10}$$

3.2 Method with coefficients depending on the frequency

We consider the five stage method of Calvo and Sanz-Serna this method has order four. We ask for the method to have phase lag order infinity and solve for b_5

$$b_5 = (A - 2\cos v)/B,$$

where

$$\begin{aligned} A &= 2 - 0.874980177205473866v^2 + 0.062496696200912311v^4 \\ &\quad -0.0015556392423006952v^6 + 9.27394413942482 * 10^{-6}v^8 \\ B &= v^2 - 0.16666666666666667v^4 + \\ &\quad 0.008596200666029143v^6 - 0.0001501637889589645v^8 \end{aligned}$$

4 Numerical results

We shall use our new methods on several test problems such as the harmonic oscillator, the inhomogeneus equation, the two coupled oscillators and the computation of the eigenvalues of the one-dimensional time-independent Schrödinger equation.

We will compare the new methods presented here (*pl8*,*pf*) with the sixth phase-lag order SRKN methods of Vyver (*Vyver3*, *Vyver4*), the classical fifth order SRKN method of Calvo and Sanz-Serna (*CSS*), the classical RKN methods of fifth and sixth algebraic order (*RKN5*, *RKN6*) ([7],page 285, [5]).

4.1 Harmonic Oscillator

We consider the following problem:

$$y'' = -v^2y, \quad y(0) = 0, \quad y'(0) = v$$

with $v = 10$. In this case the exact solution is

$$y(x) = \sin(vx),$$

For this problem we use $w = 10$. The problem has been solved numerically in the interval $[0,1000]$ with steps $h = 0.1$ and $h = 0.05$. In Table 1 we present the maximum absolute error of the solution.

Table 1: *Maximum Absolute Error for the Harmonic Oscillator*

	*Vyver*3	*Vyver*4	*pl*8	*pf*
$h=0.1$	$2.91\,10^{-1}$	$7.57\,10^{-2}$	$6.15\,10^{-3}$	$3.67\,10^{-4}$
$h=0.05$	$4.031\,01^{-3}$	$1.08\,10^{-3}$	$3.19\,10^{-4}$	$1.79\,10^{-5}$

Table 1 (continued): *Maximum Absolute Error for the Harmonic Oscillator*

	CSS	*RKN*5	*RKN*6
$h=0.1$	$7.32\,10^{-1}$	$--$	$2.14\,10^{-4}$
$h=0.05$	$4.62\,10^{-2}$	$9.08\,10^{-2}$	$2.45\,10^{-4}$

4.2 Inhomogeneous Equation

We consider the following problem:

$y'' = -v^2 y + (v^2-1)sinx, \quad y(0)=1, \quad y'(0)=v+1$

where $x \geq 0$ and $v = 10$. The exact solution is

$y(x) = \cos(vx) + \sin(vx) + \sin(x),$

For this problem we use $w = 10$. The problem has been solved numerically in the interval $[0,1000]$ with steps $h = 0.1$ and $h = 0.05$. In Table 2 we present the maximum absolute error.

Table 2: *Maximum Absolute Error for the inhomogeneous*

	*Vyver*3	*Vyver*4	*pl*8	*pf*
$h=0.1$	0.41	0.11	$3.57\,10^{-3}$	$5.04\,10^{-4}$
$h=0.5$	$5.55\,10^{-3}$	$1.46\,10^{-3}$	$2.71\,10^{-4}$	$2.22\,10^{-5}$

Table 2 (continued): *Maximum Absolute Error for the inhomogeneous*

	CSS	*RKN*5	*RKN*6
$h=0.1$	$--$	$--$	$2.33\,10^{-2}$
$h=0.5$	$6.542\,10^{-2}$	0.13	$3.47\,10^{-4}$

4.3 Two coupled oscillators with different frequencies

$y_1'' = -y_1 + 2\varepsilon y_1 y_2, \quad y_1(0)=1, \quad y_1'(0)=0,$
$y_2'' = -2y_2 + \varepsilon y_1^2 + 4\varepsilon y_2^3, \quad y_2(0)=1, \quad y_2'(0)=0$

We choose $\varepsilon = 10^{-4}$ and use as reference solution $y_1(10^3) = 0.56242453952476$ and $y_2(10^3) = 0.92464439359914$ For this problem we use $w_1 = 1$ and $w_2 = \sqrt{2}$.

Table 3: *Absolute Error at the end point for the coupled oscillators*

	*Vyver*3	*Vyver*4	*pl*8	*pf*
$h=1$	$2.48\,10^{-2}$	$6.20\,10^{-3}$	$1.65\,10^{-3}$	$1.09\,10^{-4}$
	$-2.23\,10^{-1}$	$4.26\,10^{-2}$	$4.38\,10^{-3}$	$3.13\,10^{-4}$
$h=0.5$	$3.48\,10^{-4}$	$8.64\,10^{-5}$	$4.13\,10^{-5}$	$3.29\,10^{-6}$
	$1.91\,10^{-2}$	$5.08\,10^{-4}$	$2.22\,10^{-5}$	$2.48\,10^{-5}$

Table 3 (continued): *Absolute Error at the end point for the coupled oscillators*

	CSS	*RKN*5	*RKN*6
$h=1$	$6.05\,10^{-2}$	$2.99\,10^{-1}$	$1.30\,10^{-3}$
	$7.46\,10^{-2}$	$--$	$5.81\,10^{-3}$
$h=0.5$	$3.82\,10^{-3}$	$6.69\,10^{-3}$	$1.99\,10^{-5}$
	$9.68\,10^{-3}$	$7.51\,10^{-2}$	$9.64\,10^{-5}$

4.4 Computation of the eigenvalues of the one-dimensional time-independent Schrödinger equation

The Schrödinger equation may be written in the form

$$\frac{d^2q}{dx^2} = -B(x)\,q \quad \text{where} \quad B(x) = 2(E - V(x)).$$

E is the energy eigenvalue, $V(x)$ the potential, and $y(x)$ the wave function.

The Hamiltonian function is defined as:

$H(q,p,x) = p^2 - L(x,q,p)$

where

$$L(x,q,p) = T - U = \frac{1}{2}p^2 - \frac{1}{2}B(x)\,q^2$$

is the Lagrange function, or

$$H(q,p,x) = \frac{p^2}{2} + \frac{1}{2}B(x)\,q^2$$

Then the Hamiltonian canonical equations are:

$$p' = -\frac{\partial H}{\partial q} = -B(x)\cdot q$$
$$q' = \frac{\partial H}{\partial p} = p$$

The tested problems are the harmonic oscillator and the exponetial potential. In the implementation of the methods $w = \sqrt{(B(x))}$ has been used.

4.4.1 The Harmonic Oscillator

The potential of the one dimensional harmonic oscillator is

$$V(x) = \frac{1}{2}kx^2$$

we consider $k = 1$. The integration interval is $[-R, R]$.

The exact eigenvalues are given by

$$E_n = n + \frac{1}{2}, \quad n = 0, 1, 2, \ldots$$

In Table 1 we give the absolute error of several eigenvalues up to E_{240} computed with step size $h = 0.1$. The integration interval ranges from $R = 5$ to $R = 24$. Both new methods give very accurate eigenvalues. In Table 2 we proceed with the computation of higher state eigenvalues up to E_{1000} with $h = 0.05$ again the new methods especially *Trig6* while the classical methods failed. For Table 2 the integration interval ranges from $R = 22$ to $R = 46$.

Table 4: *Absolute Error* ($\times 10^{-6}$) *of the eigenvalues of the harmonic oscillator with step size* $h = 0.05$.

	Vyver4	pl8	pf	CSS	RKN5	RKN6
E_{10}	0	0	0	2	0	0
E_{50}	4	2	0	149	66	7
E_{100}	50	3	0	1179	1026	11
E_{150}	256	4	1	3977	5128	57
E_{200}	829	23	1	9441	–	181
E_{250}	2081	90	1	–	–	446
E_{300}	–	248	2	–	–	935

The phase-fitted method has superior performance with error smaller than 10^{-5} up to the eigenvalue $E = 1400.5$, and less than 10^{-4} up to the eigenvalue $E = 1800.5$.

4.4.2 The Exponential Potential

The exponential potential is

$$V(x) = exp(x)$$

with boundary conditions $\psi(x_{min}) = 0$ and $\psi(x_{max}) = 0$. We have used 50 points in the interval of integration $[0, \pi]$.

Table 5: *The absolute error* ($\times 10^{-6}$) *of the eigenvalues of the exponential potential.*

	Vyver4	pl8	pf	CSS	RKN5	RKN6
4.8966694	0	0	0	0	0	0
16.019267	0	1	0	3	0	0
32.263707	3	2	0	41	6	0
56.181594	13	9	3	281	97	1
88.132119	56	52	13	1243	757	8
128.10502	228	144	34	–	3817	41
176.08900	815	361	81	–	14549	164
232.07881	2506	700	147	–	–	511
296.07196	6902	1151	263	–	–	1418
368.06713	17245	1503	426	–	–	3512

5 Conclusions

In this work two new symplectic Runge-Kutte-Nystrom methods with phase lag order eight and infinity have been constructed and tested. The performance of the new methods on the harmonic oscillator, the inhomogeneous equation two coupled oscillators is more accurate (by one decimal digits) than the fourth order method of Vyver and the phase-fitted method is more accurate (by one decimal digits) than the new eigth phase-lag order method. On the computation of the eigenvalues of the Schrödinger equation for both potentials presented here the new methods have superior performance than all methods tested. For the harmonic oscillator potential the error is less than 10^{-4} for as lagre eigenvalue as E_{1800}.

References

[1] Z. A. Anastassi, T.E. Simos, A dispersive-fitted and dissipative-fitted explicit Runge-Kutta method for the numerical solution of orbital problems, *New Astronomy*, **10** (2004) 31-37.

[2] L. Brusa, L.Nigro, A one-step method for direct integration of structural dynamic equations, *International Journal for Numerical Methods in Engineering*, **14** (1980) 685-699.

[3] M.P. Calvo, J.M. Sanz-Serna, *Order Conditions for Canonical Runge-Kutta-Nyström methods*, BIT, **32** (1992) 131-142.

[4] J.R. Dormand and P.J. Prince, Runge-Kutta-Nyström Triples, *Comp. Math. Applic.*, **12** (1987) 937-949.

[5] J.R. Dormand, M.E. El-Mikkawy and P.J. Prince, Families of Runge-Kutta-Nyström Formulae, *IMA Journal of Numerical Analysis* **7** (1987) 235-250.

[6] J.R. Dormand, M.E. El-Mikkawy, P.J. Prince, High-Order Embeded Runge-Kutta-Nystrom Formulae, *IMA Journal of Numerical Analysis* **7** (1987) 423-430.

[7] Hairer E., Lubich Ch., Wanner G., *Geometric Numerical Integration*, Springer-Verlag, 2002.

[8] Th. Monovasilis, Z. Kalogiratou, T. E. Simos, Symplectic Partitioned Runge-Kutta Methods with minimal phase-lag, *Computer Physics Communication*, **181** (2010) 1251-1254.

[9] A.D. Raptis, T.E. Simos, A four step phase-fitted method for the numerical integration of second order initial-value problems,*BIT* **31** (1991) 160-168.

[10] Ruth R.D., A canonical integration technique, *IEEE Transactions on Nuclear Science*, NS **30** (1983), 2669-2671.

[11] Sanz-Serna, J.M., Calvo, M.P., *Numerical Hamiltonian Problem*, Chapman and Hall, London, 1994.

[12] T.E. Simos, Exponentially fitted Runge-Kutta-Nyström method for the numerical solution of initial-value problems with oscillating solutions, *Applied Mathematics Letters* **15** (2002) 217-225.

[13] T.E. Simos, J. Vigo-Aguiar, Exponentially fitted symplectic integrator,*Physics Review E* **67** (2003) 016701(1)-016701(7).

[14] A. Tocino and J.V. Aguiar, Symplectic Conditions for Exponential Fitting Runge-Kutta-Nyström methods, *Mathematical and Computer Modelling* , **42** (2005) 873-876.

[15] P.J. Van Der Houwen, B.P. Sommeijer, Explicit Runge-Kutta(-Nyström) methods with reduced phase errors for computing oscillating solutions, *SIAM Journal of Numerical Analysis*, **24** (1987) 595-617.
[16] Hans Van de Vyver, A symplectic exponentially fitted modified Runge-Kutta-Nyström method for the numerical integration of orbital problems, *New Astronomy*, **10** (2005) 261-269.
[17] H. Van de Vyver, A symplectic Runge-Kutta-Nyström method with minimal phase-lag, *Physics Letters A*, **367** (2007) 16-24.
[18] H. Van de Vyver, Fourth order symplectic integration with reduced phase error, *International Journal of Modern Physics C*, **19** (2008) 1257-1268.
[19] J. Vigo-Aguiar, T. E. Simos, A. Tocino, An adapted symplectic integrator for Hamiltonian systems, *International Journal of Modern Physics C* , **12** (2001) 225-234.
[20] Z. A. Anastassi, T. E. Simos, An optimized Runge-Kutta method for the solution of orbital problems, *Journal of Computational and Applied Mathematics*, **175** 1-9 (2005)
[21] Ch. Tsitouras, A Tenth Order Symplectic Runge-Kutta-Nystrm Method, *Celestial Mechanics and Dynamical Astronomy* **74**, 223-230 (1999).
[22] G Psihoyios, TE Simos, A fourth algebraic order trigonometrically fitted predictorcorrector scheme for IVPs with oscillating solutions, *Journal of Computational and Applied Mathematics*, **175**, 137-147 (2005).
[23] A. D. Raptis, T. E. Simos, A four-step phase-fitted method for the numerical integration of second order initial-value problems, *BIT Numerical Mathematics*, **31**, 160-168 (1991).
[24] T Allahviranloo, N Ahmady, E Ahmady, Numerical solution of fuzzy differential equations by predictor-corrector method, *Information Sciences*, **177**, 1633-1647 (2007).
[25] T. E. Simos, Optimizing a Hybrid Two-Step Method for the Numerical Solution of the Schrödinger Equation and Related Problems with Respect to Phase-Lag, *Journal of Applied Mathematics*, Article ID 420387, doi:10.1155/2012/420387, **2012** (2012).
[26] T.E. Simos, New Stable Closed Newton-Cotes Trigonometrically Fitted Formulae for Long-Time Integration, *Abstract and Applied Analysis*, Article Number: 182536, DOI: 10.1155/2012/182536(2012)
[27] A. Konguetsof and T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrodinger equation, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS*, **158**, 93-106 (2003)
[28] Z. Kalogiratou, T. Monovasilis and T.E. Simos, Symplectic integrators for the numerical solution of the Schrodinger equation, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* **158**, 83-92 (2003)
[29] Z. Kalogiratou and T.E. Simos, Newton-Cotes formulae for long-time integration, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS*, **158**, 75-82(2003)
[30] G. Psihoyios and T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* **158**, 135-144 (2003)
[31] T.E. Simos, I.T. Famelis and C. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions, *NUMERICAL ALGORITHMS* **34**, 27-40 (2003)
[32] T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution, *APPLIED MATHEMATICS LETTERS*, **17**, 601-607 (2004)
[33] K. Tselios and T.E. Simos, Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS*, **175**, 173-181 (2005)
[34] D.P. Sakas and T.E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase-lag for the numerical solution of the radial Schrodinger equation, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* **175**, 161-172 (2005)
[35] G. Psihoyios and T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* **175**, 137-147 (2005)
[36] Z. A. Anastassi and T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems, *JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS* **175**, 1-9 (2005)
[37] T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems, *APPLIED MATHEMATICS LETTERS* **22**, 1616-1621 (2009)
[38] S. Stavroyiannis and T.E. Simos, Optimization as a function of the phase-lag order of nonlinear explicit two-step P-stable method for linear periodic IVPs, *APPLIED NUMERICAL MATHEMATICS* **59**, 2467-2474 (2009)
[39] T.E. Simos, Exponentially and Trigonometrically Fitted Methods for the Solution of the Schrodinger Equation, *ACTA APPLICANDAE MATHEMATICAE* **110**, 1331-1352 (2010)
[40] T. E. Simos, New Stable Closed Newton-Cotes Trigonometrically Fitted Formulae for Long-Time Integration, *Abstract and Applied Analysis*, **2012**, Article ID 182536, 15 pages, doi:10.1155/2012/182536
[41] Z.A. Anastassi and T.E. Simos, A parametric symmetric linear four-step method for the efficient integration of the Schrodinger equation and related oscillatory problems, *Journal of Computational and Applied Mathematics*, **236** (2012) 3880-3889
[42] A.A. Kosti, Z.A. Anastassi and T.E. Simos, An optimized explicit Runge-Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems, *J. Math. Chem.* **47** 315-330 (2010)
[43] Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation *J. Math. Chem* **37** 281-293 (2005)
[44] Z.A. Anastassi, T.E. Simos, A family of exponentially-fitted Runge-Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation, *J. Math. Chem* **41** 79-100 (2007)
[45] Ch. Tsitouras, I.Th. Famelis and T.E. Simos, On Modified Runge-Kutta Trees and Methods, *Computers & Mathematics with Applications* **62** 2101-2111 (2011)
[46] T.E. Simos, I.T. Famelis and C. Tsitouras, Zero Dissipative, Explicit Numerov-Type Methods for second order IVPs

with Oscillating Solutions, *Numerical Algorithms*, **34**, 27-40 (2003)
[47] D.P. Sakas, T.E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation, *J. Math. Chem* **37** 317-331 (2005)
[48] T.E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **46** 981-1007 (OCT 2009)
[49] T.E. Simos, A two-step method with vanished phase-lag and its first two derivatives for the numerical solution of the Schrödinger equation, *Journal of Mathematical Chemistry* **49** 2486-2518 (2011)
[50] T.E. Simos, New high order multiderivative explicit four-step methods with vanished phase-lag and its derivatives for the approximate solution of the Schrödinger equation. Part I: Construction and theoretical analysis, *Journal of Mathematical Chemistry* **51** 194-226 (2013)
[51] K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation, *J. Math. Chem* **34** 83-94 (2003)
[52] K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrodinger equation, *J. Math. Chem* **35** 55-63 (2004)
[53] T. Monovasilis and T.E. Simos, New second-order exponentially and trigonometrically fitted symplectic integrators for the numerical solution of the time-independent Schrödinger equation, *J. Math. Chem* **42** 535-545 (2007)
[54] T. Monovasilis, Z. Kalogiratou , T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation *J. Math. Chem* **37** 263-270 (2005)
[55] T. Monovasilis, Z. Kalogiratou , T.E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation, *J. Math. Chem* **40** 257-267 (2006)
[56] T.E. Simos, High order closed Newton-Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation, *Appl. Math. Comput.* **209** 137-151 (2009)
[57] T.E. Simos, Closed Newton-Cotes Trigonometrically-Fitted Formulae for the Solution of the Schrödinger Equation, *MATCH Commun. Math. Comput. Chem.* **60** 787-801 (2008)
[58] T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for the numerical integration of the Schrödinger equation, *J. Math. Chem.* **44** 483-499 (2008)
[59] T.E. Simos, New Closed Newton-Cotes Type Formulae as Multilayer Symplectic Integrators, *Journal Of Chemical Physics* **133** Article Number: 104108 (2010)
[60] T.E. Simos, High order closed Newton-Cotes exponentially and trigonometrically fitted formulae as multilayer symplectic integrators and their application to the radial Schrödinger equation, *J. Math. Chem* **50** 1224-1261 (2012)
[61] Z. Kalogiratou, Th. Monovasilis and T.E. Simos, New modified Runge-Kutta-Nyström methods for the numerical integration of the Schrödinger equation, *Computers & Mathematics with Applications* **60** 1639-1647 (2010)
[62] T.E. Simos, A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems *J. Math. Chem* **34** 39-58 JUL 2003
[63] T.E. Simos, Exponentially - fitted multiderivative methods for the numerical solution of the Schrödinger equation, *J. Math. Chem* **36** 13-27 (2004)
[64] T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation, *J. Math. Chem* **40** 305-318 (2006)
[65] T.E. Simos, A family of four-step trigonometrically-fitted methods and its application to the Schrodinger equation *J. Math. Chem* **44** 447-466 (2009)
[66] Z.A. Anastassi and T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution *J. Math. Chem* **45** 1102-1129 (2009)
[67] G. Psihoyios, T.E. Simos, Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation, *J. Math. Chem* **37** 295-316 (2005)
[68] G. Psihoyios, T.E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order Predictor-Corrector methods, *J. Math. Chem* **40** 269-293 (2006)
[69] Z.A. Anastassi and T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution, *J. Math. Chem.* **45** 1102-1129 (2009)
[70] G.A. Panopoulos, Z.A. Anastassi and T.E. Simos, Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions, *J. Math. Chem.* **46** 604-620 (2009)
[71] Ibraheem Alolyan and T. E. Simos, A new four-step hybrid type method with vanished phase-lag and its first derivatives for each level for the approximate integration of the Schrödinger equation, *Journal of Mathematical Chemistry*, **51** 2542-2571 (2013)
[72] Ibraheem Alolyan and T. E. Simos, A RungeKutta type four-step method with vanished phase-lag and its first and second derivatives for each level for the numerical integration of the Schrödinger equation, *Journal of Mathematical Chemistry*, **52** 917-947 (2014)
[73] Ibraheem Alolyan and T. E. Simos, A new four-step Runge-Kutta type method with vanished phase-lag and its first, second and third derivatives for the numerical solution of the Schrödinger equation, *Journal of Mathematical Chemistry*, **51** 1418-1445 (2013)
[74] Ibraheem Alolyan and T. E. Simos, High order four-step hybrid method with vanished phase-lag and its derivatives for the approximate solution of the Schrödinger equation, *Journal of Mathematical Chemistry*, **51** 532-555 (2013)
[75] Ibraheem Alolyan and T. E. Simos, A new high order two-step method with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation, *Journal of Mathematical Chemistry*, **50** 2351-2373 (2012)
[76] Ibraheem Alolyan and T. E. Simos, A new hybrid two-step method with vanished phase-lag and its first and second derivatives for the numerical solution of the Schrödinger equation and related problems, *Journal of Mathematical Chemistry*, **50** 1861-1881 (2012)
[77] Ibraheem Alolyan and T. E. Simos, New open modified trigonometrically-fitted Newton-Cotes type multilayer symplectic integrators for the numerical solution of the Schrödinger equation, *Journal of Mathematical Chemistry*, **50** 782-804 (2012)

[78] I. Alolyan, Z.A. Anastassi and T. E. Simos, A new family of symmetric linear four-step methods for the efficient integration of the Schrödinger equation and related oscillatory problems, *APPLIED MATHEMATICS AND COMPUTATION*, **218** 5370-5382 (2012)
[79] Ibraheem Alolyan and T. E. Simos, A family of high-order multistep methods with vanished phase-lag and its derivatives for the numerical solution of the Schrödinger equation, *COMPUTERS & MATHEMATICS WITH APPLICATIONS*, **62** 3756-3774 (2011)
[80] Ibraheem Alolyan and T. E. Simos, A family of ten-step methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation, *Journal of Mathematical Chemistry*, **49** 1843-1888 (2011)
[81] A.A. Kosti, Z.A. Anastassi and T. E. Simos, Construction of an optimized explicit Runge-Kutta-Nyström method for the numerical solution of oscillatory initial value problems, *COMPUTERS & MATHEMATICS WITH APPLICATIONS*, **61** 3381-3390 (2011)
[82] Ibraheem Alolyan and T. E. Simos, A family of eight-step methods with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation, *Journal of Mathematical Chemistry*, **49** 711-764 (2011)
[83] Ibraheem Alolyan and T. E. Simos, On Eight-Step Methods with Vanished Phase-Lag and Its Derivatives for the Numerical Solution of the Schrödinger equation, *MATCH-COMMUNICATIONS IN MATHEMATICAL AND IN COMPUTER CHEMISTRY*, **66** 473-546 (2011)
[84] Ibraheem Alolyan and T. E. Simos, High algebraic order methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation, *Journal of Mathematical Chemistry*, **48** 925-958 (2010)
[85] Ibraheem Alolyan and T. E. Simos, Mulitstep methods with vanished phase-lag and its first and second derivatives for the numerical integration of the Schrödinger equation, *Journal of Mathematical Chemistry*, **48** 1092-1143 (2010)

Zacharoula Kalogiratou (b. 1966 in Athens, Greece) is a Professor at the Department of Informatics and Computer Technology of the Technological Educational Institute of Western Macedonia at Kastoria, Greece. She is a graduate of the Mathematics Department (1987) of the University of Athens, holds a Master's degree in Numerical Analysis and Computing (1989) from the Department of Mathematics of the University of Manchester and Ph.D. in Numerical Analysis (1992) from the University of Manchester, U.K. Her research interests are in numerical analysis and specifically in numerical solution of differential equations. She is the author of over 40 peer-reviewed publications and she is referee in scientific journals and conferences.

Theodoros Monovasilis (b. 1969 in Kastoria, Greece) is an Associate Professor at the Department of International Trade of the Technological Educational Institute of Western Macedonia at Kastoria Greece since March 2008 as well as collaborator from 1996. Dr Monovasilis received his B.Sc. degree in Mathematics from the University of Ioannina, Greece, in 1992. He studied Applied Mathematics on postgraduate level in Democritus University of Thrace-Greece in 2002. In 2006 he received his Ph.D. degree in Applied Mathematics of the University of Peloponnese (2006). He has participated in various research programs of the Technological Educational Institute of Western Macedonia with object the Applied Mathematics and Numerical Analysis. His research interests focus on Applied Mathematics and more specifically in the numerical solution of differential equations. He is the author of over 40 peer-reviewed publications in these areas and he is referee in scientific journals and conferences.

Theodore E. Simos (b. 1962 in Athens, Greece) is a Visiting Professor within the Distinguished Scientists Fellowship Program at the Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia and Professor at the Laboratory of Computational Sciences of the Department of Computer Science and Technology, Faculty of Sciences and Technology, University of Peloponnese, GR-221 00 Tripolis, Greece. He holds a Ph.D. on Numerical Analysis (1990) from the Department of Mathematics of the National Technical University of Athens, Greece. He is Highly Cited Researcher in Mathematics http://isihighlycited.com/ and http://highlycited.com/, Active Member of the European Academy of Sciences and Arts, Active Member of the European Academy of Sciences and Corresponding Member of European Academy of Sciences, Arts and Letters. He is Editor-in-Chief of three scientific journals and editor of more than 25 scientific journals. He is reviewer in several other scientific journals and conferences. His research interests are in numerical analysis and specifically in numerical solution of differential equations, scientific computing and optimization. He is the author of over 400 peer-reviewed publications and he has more than 2000 citations (excluding self-citations).