Applied Mathematics & Information Sciences
An International Journal

http://dx.doi.org/10.12785/amis/090430

Construction of Exponentially Fitted Symplectic Runge-Kutta-Nyström Methods from Partitioned Runge-Kutta Methods

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

[1] Department of International Trade, Technological Educational Institution of Western Macedonia at Kastoria, Kastoria, P.O. Box. 30, 52100 Greece.
[2] Department of Informatics and Computer Technology, 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 and Laboratory of Computational Sciences, Department of Computer Science and Technology, University of Peloponnese, GR-221 00 Tripolis, Greece.

Received: 31 Oct. 2014, Revised: 31 Jan. 2015, Accepted: 1 Feb. 2015
Published online: 1 Jul. 2015

Abstract: In this work we derive exponentially fitted symplectic Runge-Kutta-Nyström (RKN) methods from symplectic exponentially fitted partitioned Runge-Kutta (PRK) methods methods. We construct RKN methods from PRK methods with up to five stages and fourth algebraic order.

Keywords: Partitioned Runge Kutta methods, Runge Kutta Nyström methods, Symplectic methods, Hamiltonian systems, Exponential fitting.

1 Introduction

The numerical solution of initial or boundary value problems with special properties is a subject of large research activity (see [1] - [96]). More specifically, numerical solution of Hamiltonian systems with symplectic single step methods has been considered by many authors in the last thirty years.

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

$$p' = f(p,q,x), \quad q' = g(p,q,x) \tag{1}$$

with

$$f(q,x) = -\frac{\partial H}{\partial q}(p,q,x),$$
$$g(p,x) = \frac{\partial H}{\partial p}(p,q,x)$$

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.

Partitioned Runge Kutta (PRK) methods appear in the literature in 1976 [4] in order to use an explicit and an implicit RK method to integrate a system of ODEs partitioned into a nonstiff and a stiff part. Recent interest for partitioned methods came up when solving Hamiltonian systems and symplectic PRK (SPRK) methods have been developed in the past thirty years starting with the work of Ruth [20], Forest and Ruth [2] who derived the order conditions using Lie formalisation. Also Abia and Sanz-Serna [1] [12] considered symplectic PRK methods and gave the order conditions using graph theory according to the formalisation of Butcher, the

* Corresponding author e-mail: monoba@kastoria.teikoz.gr, kalogira@kastoria.teikoz.gr, tsimos.conf@gmail.com

theory of these methods can be found in the book of SanzSerna and Calvo [21].

We shall consider systems with separable Hamiltonian

$$H(p,q,x) = T(p,x) + V(q,x)$$

where T is the kinetic energy and V is the potential energy. In many cases the kinetic energy has the special quadratic form

$$T(p) = \frac{1}{2} p^T p.$$

Then the system (1) can be written as:

$$p' = f(q,x), \quad q' = p \tag{2}$$

where

$$f(q,x) = -\frac{\partial V}{\partial q}(q,x).$$

The Hamiltonian system (2) can be written as a system of second order ODEs

$$q'' = f(q,x), \quad \text{where} \quad f(q,x) = -\frac{\partial}{\partial q} V(q,x). \tag{3}$$

Symplectic Runge-Kutta-Nyström (SRKN) methods are appropriate methods for the numerical integration of such systems.

The solution of Hamiltonian systems often has oscillatory or periodic behavior and methods that take into acount this behavior have been developed. Among these methods are exponetially/trigonometrically (EF/TF) fitted methods with variable coefficients depending on the frequency of the specific problem. The idea of combining symplecticity with exponential fitting was first introduced by Vigo-Aguiar et. al. in [28] they have constructed an adaptive EFSRKN method and Simos and Vigo-Aguiar [23] they presented a two stages modified second order EFSRKN.

The authors in a series of works developed EFSPRK methods ([5], [7], [9], [10], [11]) and symplectic conditions for EFSPRK methods have been given. Also in [6] a survey of SPRK methods with special properties for the solution of problems with oscillatory or periodic behavior has been presented, these methods are of order up to fifth with six stages.

The construction of EFSRKN methods was also considered by Van de Vyver [25] who constructed a second order method with two stages where the fitting is done at each stage. Tocino and Vigo-Aguiar [24] gave symplectic conditions for EFSRKN methods without giving a specific method. Franco [3] constructed a second and a fourth order EFSRKN method with three stages. The construction of EFSRKN methods is a difficult procedure since the symplecticity conditions together with the exponentially fitting conditions are very complicated. For this reason methods of higher order have not been developed.

In this work for first time in the literature we derive EFSRKN methods from EFSPRK methods. In section 2 the theory of PRK and RKN methods is given. In section 3 we present how the second order EFSRKN method with two stages presented in [25] can be derived by a EFSPRK method developed by the authors in [6] and we construct a family of second order methods with three stages.

2 Classical RKN and PRK methods

An s-stage Partitioned Runge Kutta method for the special Hamiltonian system (2) is

$$\begin{aligned} p_{n+1} &= p_n + h \sum_{i=1}^{s} c_i f(x_n + C_i h, Q_i), \\ q_{n+1} &= q_n + h \sum_{i=1}^{s} d_i P_i, \\ P_i &= p_n + h \sum_{j=1}^{s} a_{ij} f(x + C_j h, Q_j), \\ Q_i &= q_n + h \sum_{j=1}^{s} A_{ij} P_j. \end{aligned} \tag{4}$$

The associated Butcher arrays are

$$\begin{array}{c|ccc} C_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ C_s & a_{s1} & \cdots & a_{ss} \\ \hline & c_1 & \cdots & c_s \end{array} \qquad \begin{array}{c|ccc} D_1 & A_{11} & \cdots & A_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ D_s & A_{s1} & \cdots & A_{ss} \\ \hline & d_1 & \cdots & d_s \end{array}$$

where

$$C_i = \sum_{j=1}^{s} a_{ij}, \quad \text{and} \quad D_i = \sum_{j=1}^{s} A_{ij}$$

Assume that the coefficients of the PRK method satisfy the relations

$$c_i A_{ij} + d_j a_{ji} - c_i d_j = 0, \quad i,j = 1,2,\ldots,s.$$

Then the method is symplectic when applied to Hamiltonian problems with separable Hamiltonian.

The advantage of using SPRK is that there exist explicit SPRK methods. Assume the explicit form $a_{ij} = 0$ for $i < j$ and $A_{ij} = 0$ for $i \le j$. Then due to the symplecticness requirement

$$a_{ij} = c_j, \quad A_{ij} = d_j, \quad C_i = \sum_{j=1}^{i} c_j, \quad D_i = \sum_{j=1}^{i-1} d_j.$$

The SPRK method can be denoted by

$$[c_1, c_2, \ldots, c_s](d_1, d_2, \ldots, d_s)$$

This implies a favourable implementation of the method using only two d-dimensional vectors:

$$\begin{aligned} P_0 &= p_n, \\ Q_1 &= q_n, \\ P_i &= P_{i-1} + h c_i f(Q_i, x_n + C_i h), \\ Q_{i+1} &= Q_i + h d_i P_i, \\ p_{n+1} &= P_s, \\ q_{n+1} &= Q_{s+1}. \end{aligned}$$

The authors considered modified PRK methods introducing the parameters $\hat{\alpha}_i$, $\hat{\beta}_i$ (see [6])

$$\begin{aligned} P_i &= \alpha_i P_{i-1} + h\hat{c}_i f(Q_i, x_n + D_i h), \\ Q_{i+1} &= \beta_i Q_i + h\hat{d}_i P_i. \end{aligned} \tag{5}$$

In order to present symplecticity the new parameters have to satisfy the condition

$$\prod_{i=1}^{s} \alpha_i \beta_i = 1 \tag{6}$$

Requiring that the method is exact for the trigonometrical functions $\sin(x)$ and $\cos(x)$ we obtain

$$\begin{aligned} \alpha_i &= \frac{\cos((C_i - D_i)v)}{\cos((C_{i-1} - D_i)v)}, \\ \beta_i &= \frac{\cos((C_i - D_{i+1})v)}{\cos((C_i - D_i)v)}, \\ \hat{c}_i &= \frac{\sin(c_i v)}{v} \frac{1}{\cos((C_{i-1} - D_i)v)}, \\ \hat{d}_i &= \frac{\sin(d_i v)}{v} \frac{1}{\cos((C_i - D_i)v)}. \end{aligned}$$

An explicit RKN method is

$$Y_i = y_n + \gamma_i h y'_n + h^2 \sum_{j=1}^{i-1} \alpha_{ij} f(x_n + \gamma_j h, Y_j), \tag{7}$$

$$y_{n+1} = y_n + h y'_n + h^2 \sum_{i=1}^{s} b_i f(x_n + \gamma_i h, Y_i),$$

$$y'_{n+1} = y'_n + h \sum_{i=1}^{s} b'_i f(x_n + \gamma_i h, Y_i),$$

and is associated with a Butcher tableau

$$\begin{array}{c|cccc} \gamma_1 & & & & \\ \gamma_2 & \alpha_{21} & & & \\ \gamma_3 & \alpha_{31} & \alpha_{32} & & \\ \vdots & \vdots & \vdots & & \\ \gamma_s & \alpha_{s1} & \alpha_{s2} & \cdots & \alpha_{s,s-1} \\ \hline & b_1 & b_2 & \cdots\ b_{s-1} & b_s \\ \hline & b'_1 & b'_2 & \cdots\ b'_{s-1} & b'_s \end{array}$$

The RKN method (7) can be derived by the PRK method (4) as follows

$$\begin{aligned} b_i &= \sum_{j=1}^{s} d_j a_{ji}, \quad b'_i = c_i, \\ \gamma_i &= D_i, \quad i = 1, \ldots, s \\ \alpha_{ij} &= \sum_{k=1}^{s} A_{ik} a_{kj}, \quad i, j = 1 \ldots s. \end{aligned}$$

A RKN method is symplectic when applied to Hamiltonian problems (3) if the coefficients satisfy

$$\begin{aligned} b_i &= b'_i(1 - c_i), \qquad 1 \le i \le s, \\ b_i(b'_j - \alpha_{ij}) &= b'_j(b_i - \alpha_{ji}), \qquad 1 \le i, j \le s. \end{aligned}$$

3 Construction of RKN methods from PRK methods

3.1 Two stages methods

Here we show how the second order EFSRKN method with two stages presented in [25] can be derived by a EFSPRK method developed by the authors in [6]. The two stages PRK method can be written as

$$\begin{aligned} P_0 &= p_n \\ Q_1 &= q_n, \\ P_1 &= P_0 + hc_1 f(x + c_1 h, Q_1), \\ Q_2 &= Q_1 + hd_1 P_1, \\ p_{n+1} &= P_1 + hc_2 f(x + (c_1 + c_2)h, Q_2), \\ q_{n+1} &= Q_2 + hd_2 P_2 \end{aligned}$$

We shall consider the classical second order symplectic PRK method of Yoshida [13] with coefficients

$$c_1 = c_2 = 1/2, \quad d_1 = 1, \quad d_2 = 0.$$

this method gives the RKN method with coefficients

$$\gamma_2 = 1, \quad \alpha_{21} = \frac{1}{2}, \quad b_1 = \alpha_{21}, \quad b_2 = 0, \quad b'_1 = b'_2 = \frac{1}{2}.$$

This is the RKN method modified in [23], [25]. The associated Butcher arrays are

$$\begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \quad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1 & 0 \end{array} \quad \rightarrow \quad \begin{array}{c|cc} 0 & & \\ 1 & 1/2 & \\ \hline & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

The TFSPRK method presented in [6] is

$$\begin{aligned} P_0 &= p_n \\ Q_1 &= q_n, \\ P_1 &= \alpha_1 P_0 + h\hat{c}_1 f(x + c_1 h, Q_1), \\ Q_2 &= \beta_1 Q_1 + h\hat{d}_1 P_1, \\ p_{n+1} &= \alpha_2 P_1 + h\hat{c}_2 f(x + (c_1 + c_2)h, Q_2), \\ q_{n+1} &= \beta_2 Q_2 + h\hat{d}_2 P_2 \end{aligned}$$

where

$$\alpha_1 = \cos(v/2), \quad \alpha_2 = \frac{1}{\alpha_1}, \quad \beta_1 = \beta_2 = 1,$$

$$\hat{c}_1 = \frac{\sin(v/2)}{v/2}, \hat{c}_2 = \frac{\tan(v/2)}{v/2}, \hat{d}_1 = \frac{\sin(v/2)}{v/2}, \hat{d}_2 = 1.$$

Substituting the P_is we derive the following RKN method

$$\begin{aligned} Q_1 &= q_n, \\ Q_2 &= \beta_1 q_n + h\alpha_1 \hat{d}_1 p_n + h^2 \hat{c}_1 \hat{d}_1 f_1, \\ q_{n+1} &= \beta_2 \beta_1 q_n + h\alpha_1 (\beta_2 \hat{d}_1 + \alpha_2 \hat{d}_2) p_n \\ &\quad + h^2 (\beta_2 \hat{d}_1 + \alpha_2 \hat{d}_2) \hat{c}_1 f_1 + h^2 \hat{c}_2 \hat{d}_2 f_2 \\ p_{n+1} &= \alpha_2 \alpha_1 p_n + h\alpha_2 \hat{c}_1 f_1 + h\hat{c}_2 f_2, \end{aligned}$$

or

$$\begin{aligned} Q_1 &= q_n, \\ Q_2 &= q_n + h\frac{\sin v}{v} p_n + h^2 \frac{1-\cos v}{v^2} f_1, \\ q_{n+1} &= q_n + h\frac{\sin v}{v} p_n + h^2 \frac{1-\cos v}{v^2} f_1 \\ p_{n+1} &= p_n + h\frac{\tan(v/2)}{v}(f_1+f_2) \end{aligned}$$

This is the modified RKN method presented in [25].

3.2 Three stages methods

The three stages PRK method can be written as

$$\begin{aligned} P_0 &= p_n \\ Q_1 &= q_n, \\ P_1 &= P_0 + hc_1 f(x+c_1 h, Q_1), \\ Q_2 &= Q_1 + hd_1 P_1, \\ P_2 &= P_1 + hc_2 f(x+(c_1+c_2)h, Q_2), \\ Q_3 &= Q_2 + hd_2 P_2, \\ p_{n+1} &= P_2 + hc_3 f(x+(c_1+c_2+c_3)h, Q_3), \\ q_{n+1} &= Q_3 + hd_3 P_3 \end{aligned}$$

We consider the family of three stages second order symplectic PRK methods proposed by McLachlan [8] with coefficients

$$c_1 = c_3 = z, c_2 = 1-2z, \quad d_1 = 1/2, d_2 = 1/2, d_3 = 0.$$

this method can be written as a RKN method with coefficients

$$\gamma_2 = \frac{1}{2}, \quad \gamma_3 = 1, \quad b_1 = z, \quad b_2 = 1-2z, \quad b_3 = z.$$

The associated Butcher arrays are

$$\begin{array}{c|ccc} z & z & 0 & \\ 1-z & z & 1-2z & \\ 1 & z & 1-2z & z \\ \hline & z & 1-2z & z \end{array} \qquad \begin{array}{c|ccc} 0 & 0 & 0 & \\ 1/2 & 1/2 & 0 & \\ 1 & 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 & 0 \end{array} \rightarrow \begin{array}{c|cc} 0 & & \\ 1/2 & z/2 & \\ 1 & z & 1/2-z \\ \hline & z & 1/2-z \\ \hline & z & 1-2z \quad z \end{array}$$

The optimal value of z suggested in [8] is

$$z = \frac{a^2+6a-2}{12a} \quad \text{where} \quad a = \left(2\sqrt{326}-36\right)^{1/3},$$

Franco in [3] considered the case $z = 1/6$ and constructed a modified TFRKN method.

Here we shall consider the general case, the three stages TF PRK method is of the form

$$\begin{aligned} P_0 &= p_n \\ Q_1 &= q_n, \\ P_1 &= \alpha_1 P_0 + h\hat{c}_1 f(x+c_1 h, Q_1), \\ Q_2 &= \beta_1 Q_1 + h\hat{d}_1 P_1, \\ P_2 &= \alpha_2 P_1 + h\hat{c}_2 f(x+(c_1+c_2)h, Q_2), \\ Q_3 &= \beta_2 Q_2 + h\hat{d}_2 P_2, \\ p_{n+1} &= \alpha_3 P_2 + h\hat{c}_3 f(x+(c_1+c_2+c_3)h, Q_3), \\ q_{n+1} &= \beta_3 Q_3 + h\hat{d}_3 P_3, \end{aligned}$$

where

$$\alpha_1 = \cos(zv), \quad \alpha_2 = 1, \quad \alpha_3 = \frac{1}{\alpha_1},$$

$$\beta_1 = \frac{\cos((z-\frac{1}{2})v)}{\cos(zv)}, \quad \beta_2 = \frac{1}{\beta_1}, \quad \beta_3 = 1,$$

$$\hat{c}_1 = \frac{\sin(zv)}{v}, \quad \hat{c}_2 = \frac{2}{v}\sin((z-\frac{1}{2})v), \quad \hat{c}_3 = \frac{\tan(zv)}{v},$$

$$\hat{d}_1 = \frac{\sin(v/2)}{(v\cos(zv))}, \quad \hat{d}_2 = \frac{\sin(v/2)}{v\cos((z-\frac{1}{2})v)}, \quad \hat{d}_3 = 0.$$

Substituting the P_is we derive the following TFRKN method

$$\begin{aligned} Q_1 &= q_n, \\ Q_2 &= \beta_1 q_n + h\alpha_1 \hat{d}_1 p_n + h^2 \hat{c}_1 \hat{d}_1 f_1, \\ Q_3 &= \beta_2\beta_1 q_n + h\alpha_1(\beta_2\hat{d}_1 + \alpha_2\hat{d}_2)p_n \\ &+ h^2\left((\beta_2\hat{d}_1 + \alpha_2\hat{d}_2)\hat{c}_1 f_1 + \hat{c}_2\hat{d}_2 f_2\right), \\ q_{n+1} &= \beta_3\beta_2\beta_1 q_n + h\alpha_1(\beta_3\beta_2\hat{d}_1 + \alpha_2(\beta_3\hat{d}_2 + \alpha_3\hat{d}_3))p_n \\ &+ h^2(\beta_3\beta_2\hat{d}_1 + \alpha_2(\beta_3\hat{d}_2 + \alpha_3\hat{d}_3))\hat{c}_1 f_1 \\ &+ h^2(\beta_3\hat{d}_2 + \alpha_3\hat{d}_3)\hat{c}_2 f_2 + h^2\hat{d}_3\hat{c}_3 f_3 \\ p_{n+1} &= \alpha_3\alpha_2\alpha_1 p_n + h(\alpha_3\alpha_2\hat{c}_1 f_1 + \alpha_3\hat{c}_2 f_2 + \hat{c}_3 f_3) \end{aligned}$$

References

[1] L. Abia, J.M. Sanz-Serna, Partitioned Runge-Kutta methods for separable Hamiltonian problems, *Math. Comput.* **60** 617-634 (1993).

[2] E. Forest, R. Ruth, Fourth order symplectic integration, *Physica D* **43** 105-117 (1990).

[3] J.M. Franco, Exponentially fitted symplectic integrators of RKN type for solving oscillatory problems, *Comp. Phys. Commun.* **177** 479-492 (2007).

[4] E. Hofer, A partially implicit method for large stiff systems of ODE's with only few equations introducing small time-constants. *SIAM J. Numer. Anal.* **13** 645-663 (1976).

[5] Z. Kalogiratou, Th. Monovasilis, and T.E. Simos, A Symplectic Trigonometrically Fitted Modified Partitioned Runge-Kutta Method for the Numerical Integration of Orbital Problems, *Applied Numerical Analysis and Computational Mathematics (ANACM)* **2** 359-364 (2005).

[6] Z. Kalogiratou, Th. Monovasilis and T. E. Simos, Symplectic Partitioned Runge-Kutta Methods for the Numerical Integration of Periodic and Oscillatory Problems, *Recent Advances in Computational and Applied Mathematics*, Pages 169-208, Springer, ISBN 978-90-481-9980-8.

[7] Z. Kalogiratou, Symplectic Trigonometrically Fitted Partitioned Runge-Kutta Methods, *Physics Letters A* **370** 1-7(2007).

[8] R. McLachlan, On the numerical integration of ordinary differential equations by symmetric composition methods, *SIAM Journal on Scientific Computing* **16** 151-168 (1995).

[9] Th. Monovasilis, Z. Kalogiratou, T. E. Simos, Trigonometrically and Exponentially fitted Symplectic Methods of third order for the Numerical Integration of the Schrödinger Equation, *Applied Numerical Analysis and Computational Mathematics (ANACM)* **2** 238-244) (2005).

[10] Th. Monovasilis and T.E. Simos, Symplectic and Trigonometrically fitted Symplectic methods of second and third order, *Physics Letters A* **354** 377-383 (2006).

[11] Th. Monovasilis, Z. Kalogiratou, T.E. Simos, A family of trigonometrically fitted partitioned Runge-Kutta symplectic methods, *Appl. Math. Comput.* **209** 91-96 (2009).

[12] J. M. Sanz Serna and L. Abia, Order conditions for canonical Runge Kutta schemes, *SIAM J. Numer. Anal.* **28** 1081-1096 (1991).

[13] H. Yoshida, Construction of higher order symplectic integrators, *Physics Letters A* **150** 262-268 (1990)

[14] Z. A. Anastassi and T.E. Simos, A parametric symmetric linear four-step method for the efficient integration of the Schrödinger equation and related oscillatory problems, *J. Comp. Appl. Math.* **236** 3880-3889 (2012)

[15] G.A. Panopoulos, Z.A. Anastassi and T.E. Simos: Two New Optimized Eight-Step Symmetric Methods for the Efficient Solution of the Schrödinger Equation and Related Problems, *MATCH Commun. Math. Comput. Chem.* **60**, 773-785 (2008)

[16] T.E. Simos and P.S. Williams, A finite-difference method for the numerical solution of the Schrdinger equation, *J. Comp. Appl. Math.* **79** 189-205 (1997).

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

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

[19] Th. Monovasilis, Z. Kalogiratou, T. E. Simos, Symplectic Partitioned Runge-Kutta Methods with minimal phase-lag, *Comp. Phys. Commun.* **181** 1251-1254 (2010).

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

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

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

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

[24] A. Tocino and J.V. Aguiar, Symplectic Conditions for Exponential Fitting Runge-Kutta-Nyström methods, *Math. Comput. Model.* **42** 873-876 (2005).

[25] Hans Van de Vyver, A symplectic exponentially fitted modified Runge-Kutta-Nyström method for the numerical integration of orbital problems, *New Astronomy* **10** 261-269 (2005).

[26] H. Van de Vyver, A symplectic Runge-Kutta-Nyström method with minimal phase-lag, *Physics Letters A* **367** 16-24 (2007).

[27] H. Van de Vyver, Fourth order symplectic integration with reduced phase error, *International Journal of Modern Physics C* **19** 1257-1268 (2008).

[28] J. Vigo-Aguiar, T. E. Simos, A. Tocino, An adapted symplectic integrator for Hamiltonian systems, *International Journal of Modern Physics C* **12** 225-234 (2001).

[29] Z. A. Anastassi, T. E. Simos, An optimized Runge-Kutta method for the solution of orbital problems, *J. Comp. Appl. Math.*, **175** 1-9 (2005)

[30] Ch. Tsitouras, A Tenth Order Symplectic Runge-Kutta-Nystrm Method, *Celestial Mechanics and Dynamical Astronomy* **74**, 223-230 (1999).

[31] G Psihoyios, TE Simos, A fourth algebraic order trigonometrically fitted predictor?corrector scheme for IVPs with oscillating solutions, *J. Comp. Appl. Math.*, **175**, 137-147 (2005).

[32] 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).

[33] T Allahviranloo, N Ahmady, E Ahmady, Numerical solution of fuzzy differential equations by predictor-corrector method, *Information Sciences*, **177**, 1633-1647 (2007).

[34] I. Alolyan, T. E Simos, Mulitstep methods with vanished phase-lag and its first and second derivatives for the numerical integration of the Schrdinger equation, *J. Math. Chem.*, **48**, 1092-1143 (2010).

[35] A. Konguetsof and T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation, *J. Comp. Appl. Math.* **158** 93-106 (2003)

[36] Z. Kalogiratou, T. Monovasilis and T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation, *J. Comp. Appl. Math.* **158** 83-92 (2003)

[37] Z. Kalogiratou and T.E. Simos, Newton-Cotes formulae for long-time integration, *J. Comp. Appl. Math.* **158** 75-82 (2003)

[38] G. Psihoyios and T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions, *J. Comp. Appl. Math.* **158** 135-144 (2003)

[39] T.E. Simos, I.T. Famelis and C. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions, *Numer. Algorithms* **34** 27-40 (2003)

[40] T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution, *Appl. Math. Lett.* **17** 601-607 (2004)

[41] K. Tselios and T.E. Simos, Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics, *J. Comp. Appl. Math.* **175** 173-181 (2005)

[42] D.P. Sakas and T.E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation, *J. Comp. Appl. Math.* **175** 161-172 (2005)

[43] G. Psihoyios and T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions, *J. Comp. Appl. Math.* **175(1)** 137-147 (2005)

[44] Z. A. Anastassi and T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems, *J. Comp. Appl. Math.* **175** 1-9 (2005)

[45] T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems, *Appl. Math. Lett.* **22** 1616-1621 (2009)

[46] 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, *Appl. Numer. Math.* **59** 2467-2474 (2009)

[47] T.E. Simos, Exponentially and Trigonometrically Fitted Methods for the Solution of the Schrödinger Equation, *Acta Appl. Math.* **110** 1331-1352 (2010)

[48] 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

[49] 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).

[50] Z.A. Anastassi and T.E. Simos, A parametric symmetric linear four-step method for the efficient integration of the Schrödinger equation and related oscillatory problems, J. Comp. Appl. Math. **236** 3880-3889 (2012)

[51] 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)

[52] 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)

[53] 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)

[54] Ch. Tsitouras, I.Th. Famelis and T.E. Simos, On Modified Runge-Kutta Trees and Methods, *Comput. Math. Appl.* **62** 2101-2111 (2011)

[55] T.E. Simos, I.T. Famelis and C. Tsitouras, Zero Dissipative, Explicit Numerov-Type Methods for second order IVPs with Oscillating Solutions, *Numer. Algorithms*, **34**, 27-40 (2003)

[56] 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)

[57] T.E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **46** 981-1007 (OCT 2009)

[58] T.E. Simos, A two-step method with vanished phase-lag and its first two derivatives for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **49** 2486-2518 (2011)

[59] 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, *J. Math. Chem.* **51** 194-226 (2013)

[60] K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation, *J. Math. Chem* **34** 83-94 (2003)

[61] 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)

[62] 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)

[63] 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)

[64] 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)

[65] 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)

[66] 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)

[67] 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)

[68] T.E. Simos, New Closed Newton-Cotes Type Formulae as Multilayer Symplectic Integrators, *Journal Of Chemical Physics* **133(10)** Article Number: 104-108 (2010)

[69] 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)

[70] Z. Kalogiratou, Th. Monovasilis and T.E. Simos, New modified Runge-Kutta-Nyström methods for the numerical integration of the Schrödinger equation, *Comput. Math. Appl.* **60** 1639-1647 (2010)

[71] 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

[72] T.E. Simos, Exponentially - fitted multiderivative methods for the numerical solution of the Schrödinger equation, *J. Math. Chem* **36** 13-27 (2004)

[73] T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation, *J. Math. Chem* **40** 305-318 (2006)

[74] T.E. Simos, A family of four-step trigonometrically-fitted methods and its application to the Schrödinger equation *J. Math. Chem* **44** 447-466 (2009)

[75] 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)

[76] 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)

[77] 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)

[78] 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)

[79] 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)

[80] 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, *J. Math. Chem.*, **51** 2542-2571 (2013)

[81] 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, *J. Math. Chem.*, **52** 917-947 (2014)
[82] 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, *J. Math. Chem.*, **51** 1418-1445 (2013)
[83] 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, *J. Math. Chem.*, **51** 532-555 (2013)
[84] 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, *J. Math. Chem.*, **50** 2351-2373 (2012)
[85] 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, *J. Math. Chem.*, **50** 1861-1881 (2012)
[86] 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, *J. Math. Chem.*, **50** 782-804 (2012)
[87] 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, *Appl. Math. Comput.*, **218** 5370-5382 (2012)
[88] 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, *Comput. Math. Appl.*, **62** 3756-3774 (2011)
[89] 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, *J. Math. Chem.*, **49** 1843-1888 (2011)
[90] 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, *Comput. Math. Appl.*, **61** 3381-3390 (2011)
[91] 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, *J. Math. Chem.*, **49** 711-764 (2011)
[92] 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 Commun. Math. Comput. Chem.*, **66** 473-546 (2011)
[93] 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, *J. Math. Chem.*, **48** 925-958 (2010)
[94] 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, *J. Math. Chem.*, **48** 1092-1143 (2010)
[95] Z.A. Anastassi and T.E. Simos, New Trigonometrically Fitted Six-Step Symmetric Methods for the Efficient Solution of the Schrodinger Equation, *MATCH Commun. Math. Comput. Chem.* **60** 733-752 (2008).
[96] TE Simos, JV Aguiar, A modified Runge-Kutta method with phase-lag of order infinity for the numerical solution of the Schrdinger equation and related problems, *Computers & chemistry*, **25**, 275-281 (2001).

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).