J Math Chem (2009) 46:1158–1171
DOI 10.1007/s10910-008-9505-1

ORIGINAL PAPER

A family of Runge-Kutta methods with zero phase-lag and derivatives for the numerical solution of the Schrödinger equation and related problems

Z. A. Anastassi · D. S. Vlachos · T. E. Simos

Received: 5 October 2008 / Accepted: 10 November 2008 / Published online: 6 January 2009

Abstract We construct a family of two new optimized explicit Runge-Kutta methods with zero phase-lag and derivatives for the numerical solution of the time-independent radial Schrödinger equation and related ordinary differential equations with oscillating solutions. The numerical results show the superiority of the new technique of nullifying both the phase-lag and its derivatives.

Keywords Phase-fitting · Derivative · Schrödinger equation · Runge-Kutta · Explicit methods

1 Introduction

Much research has been done on the numerical integration of the radial Schrödinger equation:

$$y''(x) = \left(\frac{l(l+1)}{x^2} + V(x) - E \right) y(x) \tag{1}$$

Z. A. Anastassi · D. S. Vlachos · T. E. Simos
Laboratory of Computer Sciences, Department of Computer Science and Technology, Faculty of Sciences and Technology, University of Peloponnese, 22 100 Tripolis, Greece

Z. A. Anastassi
e-mail: zackanas@uop.gr

D. S. Vlachos
e-mail: dvlachos@uop.gr

T. E. Simos (✉)
26 Menelaou Street, Amfithea - Paleon Faliron, 175 64 Athens, Greece
e-mail: tsimos.conf@gmail.com; tsimos@mail.ariadne-t.gr

where $\frac{l(l+1)}{x^2}$ is the *centrifugal potential*, $V(x)$ is the *potential*, E is the *energy* and $W(x) = \frac{l(l+1)}{x^2} + V(x)$ is the *effective potential*. It is valid that $\lim_{x\to\infty} V(x) = 0$ and therefore $\lim_{x\to\infty} W(x) = 0$.

Many problems in chemistry, physics, physical chemistry, chemical physics, electronics etc., are expressed by Eq. 1.

In this paper we will study the case of $E > 0$. We divide $[0, \infty]$ into subintervals $[a_i, b_i]$ so that $W(x)$ is a constant with value $\bar{W}_i$. After this the problem (1) can be expressed by the approximation

$$\begin{aligned} &y_i'' = (\bar{W} - E)\, y_i, \qquad \text{whose solution is} \\ &y_i(x) = A_i\, \exp\left(\sqrt{\bar{W} - E}\, x\right) + B_i\, \exp\left(-\sqrt{\bar{W} - E}\, x\right), \\ &A_i,\ B_i\ \in \mathbb{R}. \end{aligned} \tag{2}$$

There has been an extended bibliography on the development and analysis of numerical methods for the efficient solution of the Schrödinger equation: see for example [1–129].

2 Basic theory

2.1 Explicit Runge-Kutta methods

An s-stage explicit Runge-Kutta method used for the computation of the approximation of $y_{n+1}(x)$, when $y_n(x)$ is known, can be expressed by the following relations:

$$\begin{aligned} y_{n+1} &= y_n + \sum_{i=1}^{s} b_i\, k_i \\ k_i &= h\, f\left(x_n + c_i h,\ y_n + h \sum_{j=1}^{i-1} a_{ij}\, k_j\right), \quad i = 1, \cdots, s \end{aligned} \tag{3}$$

where in this case $f\,(x, y(x)) = (W(x) - E)\ y(x)$.

Actually to solve the second order ODE (1) using first order numerical method (3), (1) becomes:

$$\begin{aligned} z'(x) &= (W(x) - E)\ y(x) \\ y'(x) &= z(x) \end{aligned} \tag{4}$$

while we use two sets of Eq. 3: one for y_{n+1} and one for z_{n+1}.

The method shown above can also be presented using the Butcher table below:

$$\begin{array}{c|cccc} 0 & & & & \\ c_2 & a_{21} & & & \\ c_3 & a_{31} & a_{32} & & \\ \vdots & \vdots & \vdots & & \\ c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} \\ \hline & b_1 & b_2 & \cdots & b_{s-1} \quad b_s \end{array} \tag{5}$$

Coefficients $c_2, \cdots, c_s$ must satisfy the equations:

$$c_i = \sum_{j=1}^{i-1} a_{ij}, \ i = 2, \cdots, s \tag{6}$$

Definition 1 [3] A Runge-Kutta method has algebraic order p when the method's series expansion agrees with the Taylor series expansion in the p first terms: $y^{(n)}(x) = y^{(n)}_{app.}(x), n = 1, 2, \cdots, p$.

A convenient way to obtain a certain algebraic order is to satisfy a number of equations derived from Tree Theory. These equations will be shown during the construction of the new methods.

2.2 Phase-lag analysis of Runge-Kutta methods

The phase-lag analysis of Runge-Kutta methods is based on the test equation

$$y' = I\omega y, \quad \omega \in R \tag{7}$$

Application of the Runge-Kutta method described in (3) to the scalar test Eq. 7 produces the numerical solution:

$$y_{n+1} = a_*^n y_n, \quad a_* = A_s(v^2) + ivB_s(v^2), \tag{8}$$

where $v = \omega h$ and A_s, B_s are polynomials in v^2 completely defined by Runge-Kutta parameters $a_{i,j}$, b_i and c_i, as shown in (5).

Definition 2 [1] In the explicit s-stage Runge-Kutta method, presented in (5), the quantities

$$t(v) = v - \arg[a_*(v)], \quad a(v) = 1 - |a_*(v)|$$

are respectively called the *phase-lag* or *dispersion error* and the dissipative error. If $t(v) = O(v^{q+1})$ and $a(v) = O(v^{r+1})$ then the method is said to be of dispersive order q and dissipative order r.

3 Construction of the new trigonometrically fitted Runge-Kutta methods

We consider the explicit Runge-Kutta method with 3 stages and 3rd algebraic order given in table (9).

$$\begin{array}{c|ccc} \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \tag{9}$$

We will construct two new optimized methods.

3.1 First optimized method with zero phase-lag

In order to develop the new optimized method, we set free b_3, while all other coefficients are borrowed from the classical method. We want the phase-lag of the method to be null, so we satisfy the equation $PL = 0$, while solving for b_3, where

$$PL = 1/6\left(6 + (-2 - 6\,b_3)\,v^2\right)\tan(v) + v^3 b_3 + 1/6\,(-5 - 6\,b_3)\,v$$

So b_3 becomes

$$b_3 = -\frac{-6\,\tan(v) + 2\,\tan(v)\,v^2 + 5\,v}{6v\left(v\tan(v) - v^2 + 1\right)}$$

and its Taylor series expansion is

$$b_3 = \frac{1}{6} - \frac{1}{30}\,v^4 - \frac{4}{315}\,v^6 + \frac{17}{2835}\,v^8 + \frac{206}{31185}\,v^{10} + \frac{7951}{12162150}\,v^{12} - \cdots$$

where $v = \omega h$, ω is a real number and indicates the dominant frequency of the problem and h is the step-length of integration.

3.2 Second optimized method with zero phase-lag and derivative

As for the development of the second optimized method, we set free b_2 and b_3, while all other coefficients are borrowed from the classical method. We want the phase-lag and its first derivative of the method to be null, so we satisfy the equations $\{PL = 0,\ PL' = 0\}$, while solving for b_2 and b_3, where

$$\begin{aligned} PL &= 1/6\left(6 + (-3\,b_2 - 6\,b_3)\,v^2\right)\tan(v) + v\left(-1/6 - b_2 - b_3 + b_3 v^2\right) \\ PL' &= -v\tan(v)\,b_2 - 2\,v\tan(v)\,b_3 + 5/6 + (\tan(v))^2 - 1/2\,v^2 b_2 \\ &\quad -1/2\,v^2 b_2\,(\tan(v))^2 + 2\,b_3 v^2 - b_3 v^2\,(\tan(v))^2 - b_2 - b_3 \end{aligned} \tag{10}$$

Then we have

$$b_2 = \frac{1}{6}\,\frac{12\,v + v^3 + \tan(v)\,v^2 - 12\,\tan(v) + v^3\,(\tan(v))^2}{v^2\left(-3\,v + \tan(v) + v\,(\tan(v))^2 - \tan(v)\,v^2 + v^3 + v^3\,(\tan(v))^2\right)}$$
$$b_3 = \frac{1}{3}\,\frac{5\,v^3\,(\tan(v))^2 + 7\,v^3 - 19\,\tan(v)\,v^2 + 6\,v\,(\tan(v))^2 - 6\,v + 6\,\tan(v)}{v^2\left(-3\,v + \tan(v) + v\,(\tan(v))^2 - \tan(v)\,v^2 + v^3 + v^3\,(\tan(v))^2\right)} \tag{11}$$

The Taylor series expansion of the coefficients are given below:

$$b_2 = \frac{2}{3} - \frac{2}{15}\,v^2 - \frac{52}{315}\,v^4 - \frac{3526}{14175}\,v^6 - \frac{173788}{467775}\,v^8 - \frac{354768808}{638512875}\,v^{10} - \cdots$$
$$b_3 = \frac{1}{6} + \frac{2}{15}\,v^2 + \frac{25}{126}\,v^4 + \frac{4201}{14175}\,v^6 + \frac{207349}{467775}\,v^8 + \frac{423287713}{638512875}\,v^{10} + \cdots \tag{12}$$

where $v = \omega h$, ω is a real number and indicates the dominant frequency of the problem and h is the step-length of integration.

4 Algebraic order of the new methods

The following 4 equations must be satisfied so that the new methods maintain the third algebraic order of the corresponding classical method (9). The number of stages is symbolized by s, where $s = 4$. Then we are presenting the Taylor series expansions of the remainders of these equations, that is the difference of the right part minus the left part.

1st Alg. Order (1 equation)	**3rd Alg. Order (4 equations)**
$\sum_{i=1}^{s} b_i = 1$	$\sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3}$
2nd Alg. Order (2 equations)	$\sum_{i,j=1}^{s} b_i a_{ij} c_j = \frac{1}{6}$
$\sum_{i=1}^{s} b_i c_i = \frac{1}{2}$	

(13)

4.1 Equations remainders for the first method

We are presenting *Rem* which is the remainder for all four equations for the first method:

$$Rem = -\frac{1}{30}\,v^4 - \frac{4}{315}\,v^6 + \frac{17}{2835}\,v^8 + \frac{206}{31185}\,v^{10} + \cdots \tag{14}$$

4.2 Equations remainders for the second method

The four remainders of the equations for the second method are:

$$
\begin{aligned}
Rem_1 &= \frac{1}{30}\,v^4 + \frac{1}{21}\,v^6 + \frac{113}{1575}\,v^8 + \frac{7171}{66825}\,v^{10} + \cdots \\
Rem_2 &= \frac{1}{15}\,v^2 + \frac{73}{630}\,v^4 + \frac{2438}{14175}\,v^6 + \frac{24091}{93555}\,v^8 + \frac{245903309}{638512875}\,v^{10} + \cdots \\
Rem_3 &= \frac{1}{10}\,v^2 + \frac{11}{70}\,v^4 + \frac{2213}{9450}\,v^6 + \frac{54634}{155925}\,v^8 + \frac{37177279}{70945875}\,v^{10} + \cdots \\
Rem_4 &= \frac{2}{15}\,v^2 + \frac{25}{126}\,v^4 + \frac{4201}{14175}\,v^6 + \frac{207349}{467775}\,v^8 + \frac{423287713}{638512875}\,v^{10} + \cdots
\end{aligned} \tag{15}
$$

We see that the two optimized methods retain the third algebraic order, since the constant term of all the remainders is zero.

5 Numerical results

5.1 The inverse resonance problem

The efficiency of the two new constructed methods will be measured through the integration of problem (1) with $l = 0$ at the interval $[0, 15]$ using the well known Woods-Saxon potential

$$
\begin{gathered}
V(x) = \frac{u_0}{1+q} + \frac{u_1\, q}{(1+q)^2}, \qquad q = \exp\left(\frac{x - x_0}{a}\right), \quad \text{where} \\
u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a}
\end{gathered} \tag{16}
$$

and with boundary condition $y(0) = 0$.

The potential $V(x)$ decays more quickly than $\frac{l\,(l+1)}{x^2}$, so for large x (asymptotic region) the Schrödinger Eq. 1 becomes

$$
y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x) \tag{17}
$$

The last equation has two linearly independent solutions $k x j_l(kx)$ and $k x n_l(kx)$, where j_l and n_l are the *spherical Bessel* and *Neumann* functions. When $x \to \infty$ the solution takes the asymptotic form

$$
\begin{aligned}
y(x) &\approx A\,k\,x\; j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\
&\approx D[sin(k\,x - \pi\,l/2) + \tan(\delta_l)\,\cos\,(k\,x - \pi\,l/2)],
\end{aligned} \tag{18}
$$

where δ_l is called *scattering phase shift* and it is given by the following expression:

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{19}$$

where $S(x) = k\,x\,j_l(k\,x)$, $C(x) = k\,x\,n_l(k\,x)$ and $x_i < x_{i+1}$ and both belong to the asymptotic region. Given the energy we approximate the phase shift, the accurate value of which is $\pi/2$ for the above problem.

We will use three different values for the energy: (i) 989.701916, (ii) 341.495874 and (iii) 163.215341. As for the frequency ω we will use the suggestion of Ixaru and Rizea [2]:

$$\omega = \begin{cases} \sqrt{E-50} & x \in [0,\ 6.5] \\ \sqrt{E} & x \in [6.5,\ 15] \end{cases} \tag{20}$$

5.2 Nonlinear problem

$y'' = -100\,y + \sin(y)$, with $y(0) = 0,\ y'(0) = 1,\ t \in [0, 20\,\pi]$, $y(20\pi) = 3.92823991 \cdot 10^{-4}$ and $\omega = 10$ as frequency of this problem.

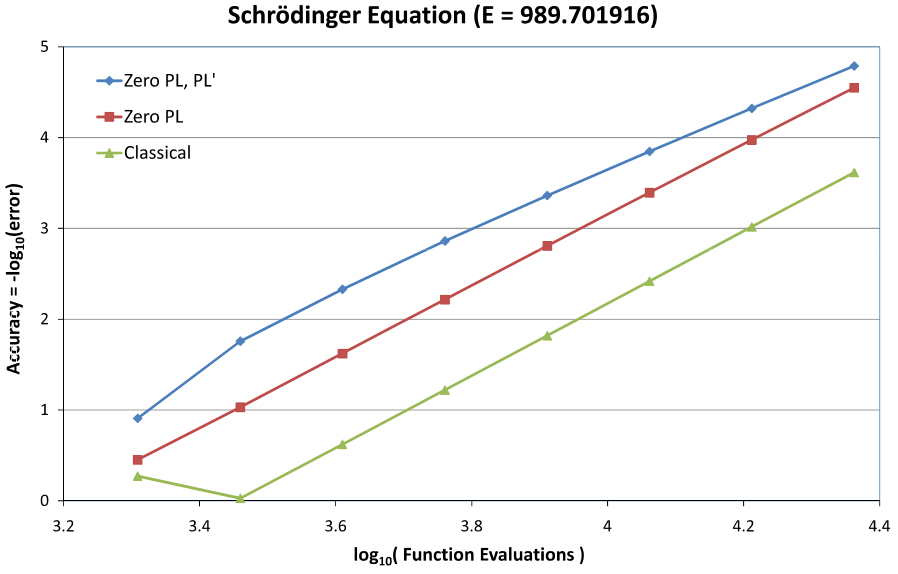

Fig. 1 Efficiency for the Schrödinger equation using $E = 989.701916$

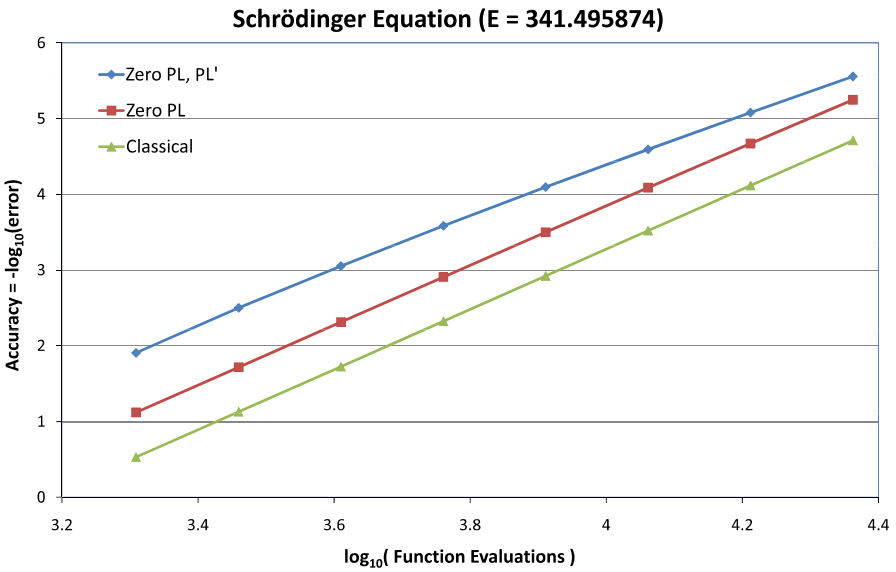

Fig. 2 Efficiency for the Schrödinger equation using $E = 341.495874$

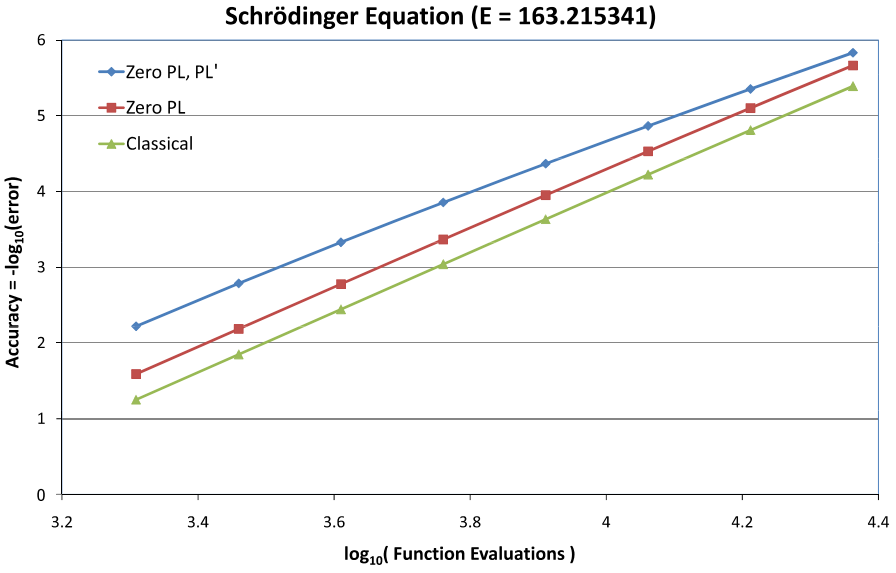

Fig. 3 Efficiency for the Schrödinger equation using $E = 163.215341$

5.3 Comparison

We present the **accuracy** of the tested methods expressed by the $-\log_{10}$(error at the end point) when comparing the phase shift to the actual value $\pi/2$ versus the $\log_{10}$(total function evaluations). The **function evaluations** per step are equal to the

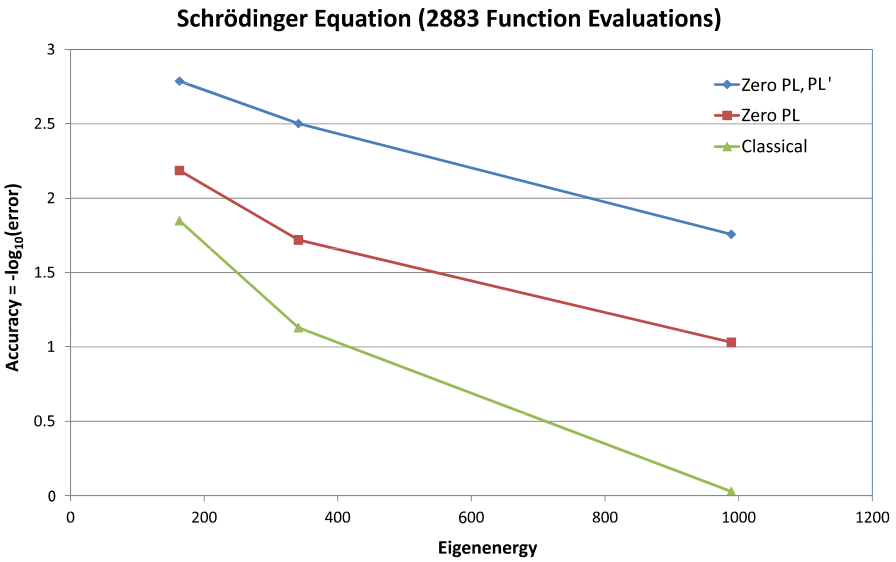

Fig. 4 Efficiency for different eigenenergies

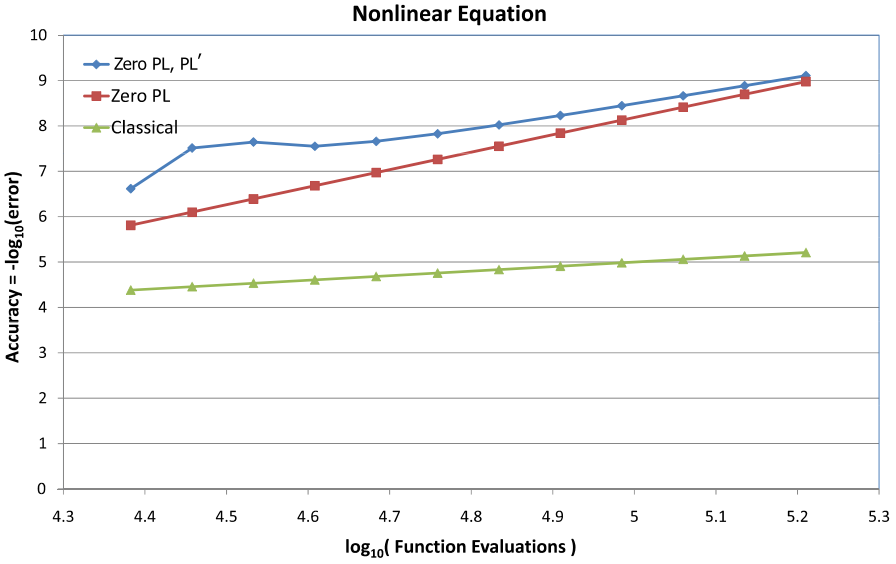

Fig. 5 Efficiency for the nonlinear problem

number of stages of the method multiplied by two that is the dimension of the vector of the functions integrated for the Schrödinger ($y(x)$ and $z(x)$). In Fig. 1 we use $E = 989.701916$, in Fig. 2 $E = 341.495874$ and in Fig. 3 $E = 163.215341$.

6 Conclusions

We compare the two optimized methods and the corresponding classical explicit Runge-Kutta method for the integration of the Schrödinger equation and the Nonlinear problem. We see that the second method with the phase-lag and its first derivative nullified is the most efficient in all cases, followed in terms of efficiency by the optimized method with zero phase-lag and then by the corresponding classical method.

References

1. T.E. Simos, in *Chemical Modelling—Applications and Theory, vol. 1: Specialist Periodical Reports, 2000* (The Royal Society of Chemistry, Cambridge, 2000), pp. 32–140
2. L.Gr. Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies. Comp. Phys. Comm. **19**, 23–27 (1980)
3. J.C. Butcher, in *Numerical Methods for Ordingary Differential Equations* (Wiley, 2003)
4. L.Gr. Ixaru, M. Micu, *Topics in Theoretical Physics* (Central Institute of Physics, Bucharest, 1978)
5. L.D. Landau, F.M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1965)
6. I. Prigogine, S. Rice (eds.), *Advances in Chemical Physics, vol. 93: New Methods in Computational Quantum Mechanics* (John Wiley & Sons, 1997)
7. G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand, Toronto, 1950)
8. T.E. Simos, in *Atomic Structure Computations in Chemical Modelling: Applications and Theory*, ed. by A. Hinchliffe (The Royal Society of Chemistry, 2000), pp. 38–142
9. T.E. Simos, Numerical methods for 1D, 2D and 3D differential equations arising in chemical problems. in *Chemical Modelling: Application and Theory*, vol. 2 (The Royal Society of Chemistry, 2002), pp. 170–270
10. T.E. Simos, P.S. Williams, On finite difference methods for the solution of the Schrödinger equation. Comput. Chem. **23**, 513–554 (1999)
11. T.E. Simos, *Numerical Solution of Ordinary Differential Equations with Periodical Solution*. Doctoral Dissertation, National Technical University of Athens, Greece, 1990 (in Greek)
12. A. Konguetsof, T.E. Simos, On the construction of exponentially-fitted methods for the numerical solution of the Schrödinger equation. J. Comput. Methods Sci. Eng. **1**, 143–165 (2001)
13. A.D. Raptis, A.C. Allison, Exponential—fitting methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **14**, 1–5 (1978)
14. A.D. Raptis, Exponential multistep methods for ordinary differential equations. Bull. Greek Math. Soc. **25**, 113–126 (1984)
15. L.Gr. Ixaru, *Numerical Methods for Differential Equations and Applications* (Reidel, Dordrecht, 1984)
16. T.E. Simos, P.S. Williams, A new Runge-Kutta-Nystrom method with phase-lag of order infinity for the numerical solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **45**, 123–137 (2002)
17. T.E. Simos, Multiderivative methods for the numerical solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **45**, 7–26 (2004)
18. A.D. Raptis, Exponentially-fitted solutions of the eigenvalue Shrödinger equation with automatic error control. Comput. Phys. Commun. **28**, 427–431 (1983)
19. A.D. Raptis, On the numerical solution of the Schrodinger equation. Comput. Phys. Commun. **24**, 1–4 (1981)
20. Z. Kalogiratou, T.E. Simos, A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation. Appl. Math. Comput. **112**, 99–112 (2000)
21. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial values problems. J. Inst. Math. Appl. **18**, 189–202 (1976)
22. A.D. Raptis, T.E. Simos, A four-step phase-fitted method for the numerical integration of second order initial-value problem. BIT **31**, 160–168 (1991)
23. P. Henrici, *Discrete Variable Methods in Ordinary Differential Equations* (John Wiley & Sons, 1962)

24. M.M. Chawla, Uncoditionally stable Noumerov-type methods for second order differential equations. BIT **23**, 541–542 (1983)
25. M.M. Chawla, P.S. Rao, A Noumerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems. J. Comput. Appl. Math. **11**(3), 277–281 (1984)
26. L.Gr. Ixaru, G. Vanden Berghe, *Exponential Fitting, Series on Mathematics and its Applications*, vol. 568 (Kluwer Academic Publisher, The Netherlands, 2004).
27. L.Gr. Ixaru, M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **38**(3), 329–337 (1985)
28. 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**(1), 79–100 (2007)
29. 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**(3), 257–267 (2006)
30. 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**(3), 269–293 (2006)
31. T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation. J. Math. Chem. **40**(3), 305–318 (2006)
32. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **37**(3), 263–270 (2005)
33. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Numerical solution of the two-dimensional time independent Schrödinger equation with Numerov-type methods. J. Math. Chem. **37**(3), 271–279 (2005)
34. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 281–293 (2005)
35. 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**(3), 295–316 (2005)
36. D.P. Sakas, T.E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 317–331 (2005)
37. T.E. Simos, Exponentially—fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
38. K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrodinger equation. J. Math. Chem. **35**(1), 55–63 (2004)
39. 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**(1–2), 39–58 (2003)
40. K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation. J. Math. Chem. **34**(1–2), 83–94 (2003)
41. J. Vigo-Aguiar J, T.E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **32**(3), 257–270 (2002)
42. G. Avdelas, E. Kefalidis, T.E. Simos, New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **31**(4), 371–404 (2002)
43. T.E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation. J. Math. Chem. **31**(2), 135–144 (2002)
44. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge-Kutta-Nystrom methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order. J. Math. Chem. **31**(2), 211–232
45. T.E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation. J. Math. Chem. **30**(1), 121–131 (2001)
46. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. J. Math. Chem. **29**(4), 281–291 (2001)
47. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results. J. Math. Chem. **29**(4), 293–305 (2001)
48. J. Vigo-Aguiar, T.E. Simos, A family of P-stable eighth algebraic order methods with exponential fitting facilities. J. Math. Chem. **29**(3), 177–189 (2001)

49. T.E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. J. Math. Chem. **27**(4), 343–356 (2000)
50. G. Avdelas, T.E. Simos, Embedded eighth order methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **26**(4), 327–341 (1999)
51. T.E. Simos, A family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **25**(1), 65–84 (1999)
52. T.E. Simos, Some embedded modified Runge-Kutta methods for the numerical solution of some specific Schrödinger equations. J. Math. Chem. **24**(1–3), 23–37 (1998)
53. T.E. Simos, Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem. J. Math. Chem. **21**(4), 359–372 (1997)
54. P. Amodio, I. Gladwell, G. Romanazzi, Numerical solution of general bordered ABD linear systems by cyclic reduction. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 5–12 (2006)
55. S.D. Capper, J.R. Cash, D.R. Moore, Lobatto-Obrechkoff formulae for 2nd order two-point boundary value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 13–25 (2006)
56. S.D. Capper, D.R. Moore, On high order MIRK schemes and Hermite-Birkhoff interpolants. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 27–47 (2006)
57. J.R. Cash, N. Sumarti, T.J. Abdulla, I. Vieira, The derivation of interpolants for nonlinear two-point boundary value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 49–58 (2006)
58. J.R. Cash, S. Girdlestone, Variable step Runge-Kutta-Nyström methods for the numerical solution of reversible systems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 59–80 (2006)
59. J.R. Cash, F. Mazzia, Hybrid mesh selection algorithms based on conditioning for two-point boundary value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 81–90 (2006)
60. F. Iavernaro, F. Mazzia, D. Trigiante, Stability and conditioning in numerical analysis. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 91–112 (2006)
61. F. Iavernaro, D. Trigiante, Discrete conservative vector fields induced by the trapezoidal method. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 113–130 (2006)
62. F. Mazzia, A. Sestini, D. Trigiante, BS linear multistep methods on non-uniform meshes. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 131–144 (2006)
63. L.F. Shampine, P.H. Muir, H. Xu, A user-friendly Fortran BVP solver. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(2), 201–217 (2006)
64. G. Vanden Berghe, M. Van Daele, Exponentially-fitted Störmer/Verlet methods. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(3), 241–255 (2006)
65. L. Aceto, R. Pandolfi, D. Trigiante, Stability analysis of linear multistep methods via polynomial type variation. JNAIAM J. Numer. Anal. Indust. Appl. Math. **2**(1–2), 1–9 (2007)
66. G. Psihoyios, A block implicit advanced step-point (BIAS) algorithm for stiff differential systems. Comput. Lett. **2**(1–2), 51–58 (2006)
67. W.H. Enright, On the use of 'arc length' and 'defect' for mesh selection for differential equations. Comput. Lett. **1**(2), 47–52 (2005)
68. T.E. Simos, P-stable four-step exponentially-fitted method for the numerical integration of the Schrödinger Equation. Comput. Lett. **1**(1), 37–45 (2005)
69. T.E. Simos, Stabilization of a four-step exponentially-fitted method and its application to the Schrödinger equation. Int. J. Mod. Phys. C **18**(3), 315–328 (2007)
70. Z. Wang, P-stable linear symmetric multistep methods for periodic initial-value problems. Comput. Phys. Commun. **171**, 162–174 (2005)
71. T.E. Simos, A Runge-Kutta Fehlberg method with phase-lag of order infinity for initial value problems with oscillating solution. Comput. Math. Appl. **25**, 95–101 (1993)
72. T.E. Simos, Runge-Kutta interpolants with minimal phase-lag. Comput. Math. Appl. **26**, 43–49 (1993)
73. T.E. Simos, Runge-Kutta-Nyström interpolants for the numerical integration of special second-order periodic initial-value problems. Comput. Math. Appl. **26**, 7–15 (1993)
74. T.E. Simos, G.V. Mitsou, A family of four-step exponential fitted methods for the numerical integration of the radial Schrödinger equation. Comput. Math. Appl. **28**, 41–50 (1994)
75. T.E. Simos, G. Mousadis, A two-step method for the numerical solution of the radial Schrödinger equation. Comput. Math. Appl. **29**, 31–37 (1995)
76. G. Avdelas, T.E. Simos, Block Runge-Kutta methods for periodic initial-value problems. Comput. Math. Appl. **31**, 69–83 (1996)
77. G. Avdelas, T.E. Simos, Embedded methods for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **31**, 85–102 (1996)

78. G. Papakaliatakis, T.E. Simos, A new method for the numerical solution of fourth order BVP's with oscillating solutions. Comput. Math. Appl. **32**, 1–6 (1996)
79. T.E. Simos, An extended Numerov-type method for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **33**, 67–78 (1997)
80. T.E. Simos, A new hybrid imbedded variable-step procedure for the numerical integration of the Schrödinger equation. Comput. Math. Appl. **36**, 51–63 (1998)
81. T.E. Simos, Bessel and Neumann fitted methods for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **42**, 833–847 (2001)
82. A. Konguetsof, T.E. Simos, An exponentially-fitted and trigonometrically-fitted method for the numerical solution of periodic initial-value problems. Comput. Math. Appl. **45**, 547–554 (2003)
83. Z.A. Anastassi, T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems. J. Comput. Appl. Math. **175**(1), 1–9 (2005)
84. G. Psihoyios, T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions. J. Comput. Appl. Math. **175**(1), 137–147 (2005)
85. D.P. Sakas, T.E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation, J. Comput. Appl. Math. **175**(1), 161–172 (2005)
86. K. Tselios, T.E. Simos, Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. J. Comput. Appl. Math. **175**(1), 173–181 (2005)
87. Z. Kalogiratou, T.E. Simos, Newton-Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
88. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 83–92 (2003)
89. A. Konguetsof, T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 93–106 (2003)
90. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**(1), 135–144 (2003)
91. Ch. Tsitouras, T.E. Simos, Optimized Runge-Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
92. T.E. Simos, An exponentially fitted eighth-order method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **108**(1–2), 177–194(1999)
93. T.E. Simos, An accurate finite difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **91**(1), 47–61 (1998)
94. R.M. Thomas, T.E. Simos, A family of hybrid exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **87**(2), 215–226 (1997)
95. Z.A. Anastassi, T.E. Simos, Special optimized Runge-Kutta methods for IVPs with oscillating solutions. Int. J. Mod. Phys. C **15**, 1–15 (2004)
96. Z.A. Anastassi, T.E. Simos, A dispersive-fitted and dissipative-fitted explicit Runge-Kutta method for the numerical solution of orbital problems. New Astron. **10**, 31–37 (2004)
97. Z.A. Anastassi, T.E. Simos, A Trigonometrically-fitted Runge-Kutta method for the numerical solution of orbital problems. New Astron. **10**, 301–309 (2005)
98. T.V. Triantafyllidis, Z.A. Anastassi, T.E. Simos, Two optimized Runge-Kutta methods for the solution of the Schrdinger equation, MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
99. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted fifth order Runge-Kutta methods for the numerical solution of the Schrödinger equation. Math. Comput. Model. **42**(7–8), 877–886 (2005)
100. Z.A. Anastassi, T.E. Simos New trigonometrically fitted six-step symmetric methods for the efficient solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
101. G.A. Panopoulos, Z.A. Anastassi, 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**, 3 (2008)
102. Z.A. Anastassi, T.E. Simos, A six-step P-stable trigonometrically-fitted method for the numerical integration of the radial Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
103. Z.A. Anastassi, 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. (in Press)
104. T.E. Simos, P.S. Williams, A finite-difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **79**(2), 189–205 (1997)

105. G. Avdelas, T.E. Simos, A generator of high-order embedded P-stable methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **72**(2), 345–358 (1996)
106. R.M. Thomas, T.E. Simos, G.V. Mitsou, A family of Numerov-type exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **67**(2), 255–270 (1996)
107. T.E. Simos, A family of 4-step exponentially fitted predictor-corrector methods for the numerical-integration of the Schrödinger-equation. J. Comput. Appl. Math. **58**(3), 337–344 (1995)
108. T.E. Simos, An explicit 4-step phase-fitted method for the numerical-integration of 2nd-order initial-value problems. J. Comput. Appl. Math. **55**(2), 125–133 (1994)
109. T.E. Simos, E. Dimas, A.B. Sideridis, A Runge-Kutta-Nyström Method for the numerical-integration of special 2nd-order periodic initial-value problems. J. Comput. Appl. Math. **51**(3), 317–326 (1994)
110. A.B. Sideridis, T.E. Simos, A low-order embedded Runge-Kutta method for periodic initial-value problems. J. Comput. Appl. Math. **44**(2), 235–244 (1992)
111. T.E. Simos, A.D. Raptis, A 4th-order Bessel fitting method for the numerical-solution of the SchrÖdinger-equation. J. Comput. Appl. Math. **43**(3), 313–322 (1992)
112. T.E. Simos, Explicit 2-step methods with minimal phase-lag for the numerical-integration of special 2nd-order initial-value problems and their application to the one-dimensional Schrödinger-equation. J. Comput. Appl. Math. **39**(1), 89–94 (1992)
113. T.E. Simos, A 4-step method for the numerical-solution of the Schrödinger-equation. J. Comput. Appl. Math. **30**(3), 251–255 (1990)
114. C.D. Papageorgiou, A.D. Raptis, T.E. Simos, A method for computing phase-shifts for scattering. J. Comput. Appl. Math. **29**(1), 61–67 (1990)
115. A.D. Raptis, Two-step methods for the numerical solution of the Schrödinger equation. Computing **28**, 373–378 (1982)
116. T.E. Simos, A new Numerov-type method for computing eigenvalues and resonances of the radial Schrödinger equation. Int. J. Mod. Phys. C-Phys. Comput. **7**(1), 33–41 (1996)
117. T.E. Simos, Predictor corrector phase-fitted methods for Y"=F(X,Y) and an application to the Schrödinger-equation. Int. J. Quantum Chem. **53**(5), 473–483 (1995)
118. T.E. Simos, Two-step almost P-stable complete in phase methods for the numerical integration of second order periodic initial-value problems. Inter. J. Comput. Math. **46**, 77–85 (1992)
119. R.M. Corless, A. Shakoori, D.A. Aruliah, L. Gonzalez-Vega, Barycentric Hermite Interpolants for event location in initial-value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 1–16 (2008)
120. M. Dewar, Embedding a general-purpose numerical library in an interactive environment. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 17–26 (2008)
121. J. Kierzenka, L.F. Shampine, A BVP Solver that Controls Residual and Error. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 27–41 (2008)
122. R. Knapp, A method of lines framework in mathematica. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 43–59 (2008)
123. N.S. Nedialkov, J.D. Pryce, Solving differential algebraic equations by taylor series (III): the DAETS code. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 61–80 (2008)
124. R.L. Lipsman, J.E. Osborn, J.M. Rosenberg, The SCHOL project at the University of Maryland: using mathematical software in the teaching of sophomore differential equations. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 81–103 (2008)
125. M. Sofroniou, G. Spaletta, Extrapolation methods in mathematica. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 105–121 (2008)
126. R.J. Spiteri, Thian-Peng Ter, pythNon: A PSE for the numerical solution of nonlinear algebraic equations. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 123–137 (2008)
127. S.P. Corwin, S. Thompson, S.M. White, Solving ODEs and DDEs with Impulses. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 139–149 (2008)
128. W. Weckesser, VFGEN: A code generation tool. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 151–165 (2008)
129. A. Wittkopf, Automatic code generation and optimization in maple. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 167–180 (2008)