J Math Chem (2010) 47:315–330
DOI 10.1007/s10910-009-9571-z

ORIGINAL PAPER

An optimized explicit Runge-Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems

A. A. Kosti · Z. A. Anastassi · T. E. Simos

Received: 14 June 2009 / Accepted: 30 June 2009 / Published online: 18 July 2009

Abstract In this paper we present an optimized explicit Runge-Kutta method, which is based on a method of Fehlberg with six stages and fifth algebraic order and has improved characteristics of the phase-lag error. We measure the efficiency of the new method in comparison to other numerical methods, through the integration of the Schrödinger equation and three other initial value problems.

Keywords Numerical solution · Initial value problems (IVPs) · Explicit methods · Runge-Kutta methods · Schrödinger equation

1 Introduction

We investigate the solution of first order differential equations of the form

$$y'(x) = f(x, y), \;\; y(x_0) = y_0, \;\; y'(x_0) = y_0'. \tag{1}$$

This type of ODE (1) appears in many areas of astronomy, astrophysics, quantum mechanics, quantum chemistry, celestial mechanics, electronics physical chemistry and chemical physics, (see [7–14]).

T. E. Simos is an active member of the European academy of sciences and arts, active member of the European academy of sciences.

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

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

An important problem that falls into this category is the radial time-independent Schrödinger equation

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

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 methods have been developed for the numerical approximation of the above problem (for more details see [1–49]).

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 (2) can be expressed by the approximation

$$\begin{aligned} & y_i'' = (\bar{W} - E)\, y_i, \qquad \text{whose solution is} \\ & y_i(x) = A_i \exp\left(\sqrt{\bar{W} - E}\, x\right) + B_i \exp\left(-\sqrt{\bar{W} - E}\, x\right), \\ & A_i,\ B_i \in \mathbb{R}. \end{aligned} \tag{3}$$

In this paper we construct an optimized explicit Runge-Kutta method based on a method of Fehlberg with 6 stages and 5th algebraic order and with constant coefficients and improved efficiency for initial value problems (IVPs) with oscillatory solution.

The paper has the following form: In Sect. 2 we present the basic theory of explicit Runge-Kutta methods, the algebraic conditions that the method must satisfy and the phase-lag analysis of the Runge-Kutta methods. In Sect. 3 we show how the new method is constructed. In Sect. 4 we present the Schrödinger equation during the resonance problem and other three IVPs that are used for the integration. We also present the methods being compared and finally in Sect. 5 we note some interesting conclusions.

2 Basic theory

2.1 Explicit Runge-Kutta methods

What is presented in this subsection is the general form of an explicit Runge-Kutta method. Furthermore, the computation of the approximate value of $y_{n+1}(x)$ in Problem 1, when $y_n(x)$ is known, is given from the following procedure:

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i\, k_i$$

$$k_i = f\left(x_n + c_i h,\ y_n + h \sum_{j=1}^{i-1} a_{ij}\, k_j \right), i = 1, \ldots, s \tag{4}$$

The upper procedure is used for the computation of the solution of Problem 1, so we have to convert this second order ODE into a system of first order ODEs. For example, for the case of problem (2) we have $f(x, y(x)) = (W(x) - E)\ y(x)$. In this way problem (2) becomes:

$$\begin{aligned} z'(x) &= (W(x) - E)\ y(x) \\ y'(x) &= z(x) \end{aligned} \tag{5}$$

An explicit Runge-Kutta method can also be presented using the Butcher table below:

$$\begin{array}{c|ccccc} 0 & & & & & \\ c_2 & a_{21} & & & & \\ c_3 & a_{31} & a_{32} & & & \\ \vdots & \vdots & \vdots & & & \\ c_s & a_{s1} & a_{s2} & \ldots & a_{s,s-1} & \\ \hline & b_1 & b_2 & \ldots & b_{s-1} & b_s \end{array} \tag{6}$$

Coefficients $c_1, c_2, \ldots, c_s$ always satisfy the equation:

$$c_i = \sum_{j=1}^{s} a_{ij},\ i = 1, \ldots, s \tag{7}$$

Definition 1 [4] A Runge-Kutta method has algebraic order p, when the method's Taylor series expansion agrees with the theoretical solution Taylor series expansion in the p first terms:

$$y^{(n)}(x) = y_n^{(n)}(x), \quad n = 1,\ 2, \ldots,\ p.$$

A Runge-Kutta method must satisfy a number of equations, in order to have a certain algebraic order. These equations are shown during the production of the methods.

2.2 Algebraic conditions

The following equations must be satisfied so that the method's algebraic order is 5:

1st Algebraic Order (1 equation)

$$\sum_{i=1}^{s} b_i = 1 \tag{8}$$

2nd Algebraic Order (2 equations in total)

$$\sum_{i=1}^{s} b_i c_i = \frac{1}{2} \tag{9}$$

3rd Algebraic Order (4 equations in total)

$$\sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3} \tag{10}$$

$$\sum_{i,j=1}^{s} b_i a_{ij} c_j = \frac{1}{6} \tag{11}$$

4th Algebraic Order (8 equations in total)

$$\sum_{i=1}^{s} b_i c_i^3 = \frac{1}{4} \tag{12}$$

$$\sum_{i,j,k=1}^{s} b_i a_{ij} a_{ik} c_k = \frac{1}{8} \tag{13}$$

$$\sum_{i,j=1}^{s} b_i a_{ij} c_j^2 = \frac{1}{12} \tag{14}$$

$$\sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk} c_k = \frac{1}{24} \tag{15}$$

5th Algebraic Order (17 equations in total)

$$\sum_{i=1}^{s} b_i c_i^4 = \frac{1}{5} \tag{16}$$

$$\sum_{i,j,k=1}^{s} b_i c_i^2 a_{ij} c_j = \frac{1}{10} \tag{17}$$

$$\sum_{i,j=1}^{s} b_i c_i a_{ij} c_j^2 = \frac{1}{15} \tag{18}$$

$$\sum_{i,j,k=1}^{s} b_i c_i a_{ij} a_{jk} c_k = \frac{1}{30} \tag{19}$$

$$\sum_{i=1}^{s} b_i a_{ij} c_j^3 = \frac{1}{20} \tag{20}$$

$$\sum_{i,j,k=1}^{s} b_i a_{ij} c_j a_{jk} c_k = \frac{1}{40} \tag{21}$$

$$\sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk} c_k^2 = \frac{1}{60} \tag{22}$$

$$\sum_{i,j=1}^{s} b_i a_{ij} a_{jk} a_{kl} c_l = \frac{1}{120} \tag{23}$$

$$\sum_{i,j,k=1}^{s} b_i a_{ij} c_j a_{ik} c_k = \frac{1}{20} \tag{24}$$

2.3 Phase-lag analysis of the Runge-Kutta methods

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

$$y' = i\, w\, y,\ i = \sqrt{-1},\ w \text{ real} \tag{25}$$

Application of this method to the scalar test equation (25) produces the numerical solution:

$$y_{n+1} = a_*^n y_n, \quad a_* = A_s(v^2) + i\, v B_s(v^2), \qquad \text{where} \quad v = w\, h \quad \text{and}$$

$$\begin{aligned} A_s(v^2) &= 1 - t_2 v^2 + t_4 v^4 + t_6 v^6 + \cdots \\ B_s(v^2) &= 1 - t_3 v^2 + t_5 v^4 + t_7 v^6 + \cdots \end{aligned} \tag{26}$$

are polynomials in v^2, completely defined by Runge-Kutta parameters $a_{i,j}$, b_i and c_i, $i = 1, \ldots, s$, $j = 1, \ldots, i-1$. y_{n+1} denotes the approximation to $y(x_{n+1})$, where $x_{n+1} = x_n + h$, $n = 0, 1, \ldots$.

A comparison of equation (26) with the solution of equation (25) leads to the following definition of the dispersion or phase-error or phase-lag:

Definition 2 [3] In the explicit s-stage Runge-Kutta method, presented in (6), the quantity

$$t(v) = v - \arg[a_*(v)],$$

is called the *phase-lag*. If $t(v) = O(v^{q+1})$, then the method is said to be of phase-lag order q.

We have the following theorem:

Theorem 1 [3] *For the Runge-Kutta method given by* (6) *and equation* (25) *we have the following formula for the direct calculation of the phase-lag order q and the phase-lag constant c:*

$$\tan(v) - v\left[\frac{B_s(v^2)}{A_s(v^2)}\right] = c v^{q+1} + O(v^{q+3})$$

3 Construction of the new method

We will consider, during the construction of the method, the computation of the phase-lag in respect to v. We consider a 6-Stage 5th algebraic order explicit Runge-Kutta method developed by Fehlberg and shown below:

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{6} & \frac{1}{6} & & & & & \\
\frac{4}{15} & \frac{4}{75} & \frac{16}{75} & & & & \\
\frac{2}{3} & \frac{5}{6} & -\frac{8}{3} & \frac{5}{2} & & & \\
\frac{4}{5} & -\frac{8}{5} & \frac{144}{25} & -4 & \frac{16}{25} & & \\
1 & \frac{361}{320} & -\frac{18}{5} & \frac{407}{128} & -\frac{11}{80} & \frac{55}{128} & \\
\hline
1 & \frac{31}{384} & 0 & \frac{1125}{2816} & \frac{9}{32} & \frac{125}{768} & \frac{5}{66}
\end{array}
\tag{27}
$$

The order of the phase-lag of the above method is 6, and is given by the formula below

$$
\begin{aligned}
\text{Phase-Lag} = {} & \frac{1}{24}\tan(v)\,v^4 - \frac{1}{540}\tan(v)\,v^6 + \tan(v) - \frac{1}{120}v^5 \\
& + \frac{1}{6}v^3 - \frac{1}{2}\tan(v)\,v^2 - v
\end{aligned}
\tag{28}
$$

and its Taylor expansion is

$$
\begin{aligned}
\text{Phase-Lag Taylor} = {} & -\frac{1}{1512}v^7 - \frac{1}{5670}v^9 - \frac{29}{415800}v^{11} \\
& - \frac{49}{1737450}v^{13} - \frac{87557}{7662154500}v^{15}
\end{aligned}
\tag{29}
$$

3.1 Construction of the new optimized method

In order to construct the new optimized method, we compute the phase-lag of the new method,which depends on v and a_{43} as given by the following relation

$$
\begin{aligned}
\text{Phase-Lag} = {} & \frac{1}{24}\tan(v)\,v^4 - \frac{1}{1350}\tan(v)\,a_{43}\,v^6 + \tan(v) - \frac{1}{120}v^5 \\
& + \frac{1}{6}v^3 - \frac{1}{2}\tan(v)\,v^2 - v
\end{aligned}
\tag{30}
$$

The Taylor series of the phase-lag in respect to v follows

$$\begin{aligned} \text{Phase-Lag Taylor} &= \left(\frac{1}{840} - \frac{1}{1350}\,a_{43}\right) v^7 + \left(\frac{1}{2268} - \frac{1}{4050}\,a_{43}\right) v^9 \\ &\quad + \left(\frac{221}{1247400} - \frac{1}{10125}\,a_{43}\right) v^{11} \\ &\quad + \left(\frac{349}{4864860} - \frac{17}{425250}\,a_{43}\right) v^{13} \\ &\quad + \left(\frac{74251}{2554051500} - \frac{31}{1913625}\,a_{43}\right) v^{15} \end{aligned} \tag{31}$$

The coefficients of the **RK-Fehlberg 5th new** depend on a_{43}.

$$\begin{array}{c|cccccc} 0 & & & & & & \\ \frac{1}{6} & \frac{1}{6} & & & & & \\ \frac{4}{15} & \frac{4}{75} & \frac{16}{75} & & & & \\ \frac{2}{3} & -\frac{2}{3}+\frac{3}{5}\,a_{43} & \frac{4}{3}-\frac{8}{5}\,a_{43} & a_{43} & & & \\ \frac{4}{5} & \frac{68}{25}-\frac{216}{125}\,a_{43} & -\frac{144}{25}+\frac{576}{125}\,a_{43} & \frac{16}{5}-\frac{72}{25}\,a_{43} & \frac{16}{25} & & \\ 1 & -\frac{827}{320}+\frac{297}{200}\,a_{43} & \frac{63}{10}-\frac{99}{25}\,a_{43} & \frac{385}{128}+\frac{99}{40}\,a_{43} & -\frac{11}{80} & \frac{55}{128} & \\ \hline 1 & \frac{31}{384} & 0 & \frac{1125}{2816} & \frac{9}{32} & \frac{125}{768} & \frac{5}{66} \end{array} \tag{32}$$

and one equation must hold in order to achieve zero factor of the v^7 term. The equation is given below

$$\frac{1}{840} - \frac{1}{1350}\,a_{43} = 0,$$

and it nullifies the coefficient of the leading term of the Taylor series expansion of the phase-lag. So we get $a_{43} = \frac{45}{28}$ and the **RK-Fehlberg 5th new** becomes

$$\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{6} & \frac{1}{6} & & & & & \\
\frac{4}{15} & \frac{4}{75} & \frac{16}{75} & & & & \\
\frac{2}{3} & \frac{25}{84} & -\frac{26}{21} & \frac{45}{28} & & & \\
\frac{4}{5} & -\frac{2}{35} & \frac{288}{175} & -\frac{10}{7} & \frac{16}{25} & & \\
1 & -\frac{443}{2240} & -\frac{9}{140} & \frac{869}{896} & -\frac{11}{80} & \frac{55}{128} & \\
\hline
1 & \frac{31}{384} & 0 & \frac{1125}{2816} & \frac{9}{32} & \frac{125}{768} & \frac{5}{66}
\end{array} \tag{33}$$

In this way we achieve to increase the order of the phase-lag of RK-Fehlberg 5th method from 6th order to 8th order. For the new method we have evaluated the remainders of equations (8–24) and they are nullified, which means that the algebraic order is preserved.

4 Numerical results

4.1 The problems

Three well-known IVPs from the literature as well as the Schrödinger Equation were chosen to test the efficiency of the constructed method.

4.1.1 Schrödinger equation-resonance problem

The efficiency of the new constructed methods will be measured through the integration of problem (2) with $l = 0$ at the interval [0, 15] using the well known Woods-Saxon potential

$$V(x) = \frac{u_0}{1+q} + \frac{u_1 q}{(1+q)^2}, \qquad q = \exp\left(\frac{x - x_0}{a}\right), \quad \text{where} \tag{34}$$
$$u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a}$$

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 equation (2) becomes

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x) \tag{35}$$

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

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D[\sin(k\,x - \pi\,l/2) + \tan(\delta_l)\,\cos(k\,x - \pi\,l/2)], \end{aligned} \tag{36}$$

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

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{37}$$

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 four different values for the energy: (1) 53.588872, (2) 163.215341, (3) 341.495874 and (4) 989.701916. As for the frequency w we will use the suggestion of Ixaru and Rizea [1]:

$$w = \begin{cases} \sqrt{E+50} & x \in [0,\ 6.5] \\ \sqrt{E} & x \in [6.5,\ 15]. \end{cases} \tag{38}$$

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 number of stages of the method multiplied by two that is the dimension of the vector of the functions integrated for the resonance problem ($y(x)$ and $z(x)$). In Fig. 1 we use $E = 53.588872$, in Fig. 2 $E = 163.215341$, in Fig. 3 $E = 341.495874$ and in Fig. 4 we use $E = 989.701916$.

4.1.2 Nonlinear problem

$$y'' = 100y + sin(y)$$

with

$$\begin{aligned} y(0) &= 0 \\ y'(0) &= 1, \quad t \in [0,\ 20\,\pi] \end{aligned} \tag{39}$$

The theoretical solution is not known, but we use $y(20\,\pi) = 3.92823991 \times 10^{-4}$ (see [2]).

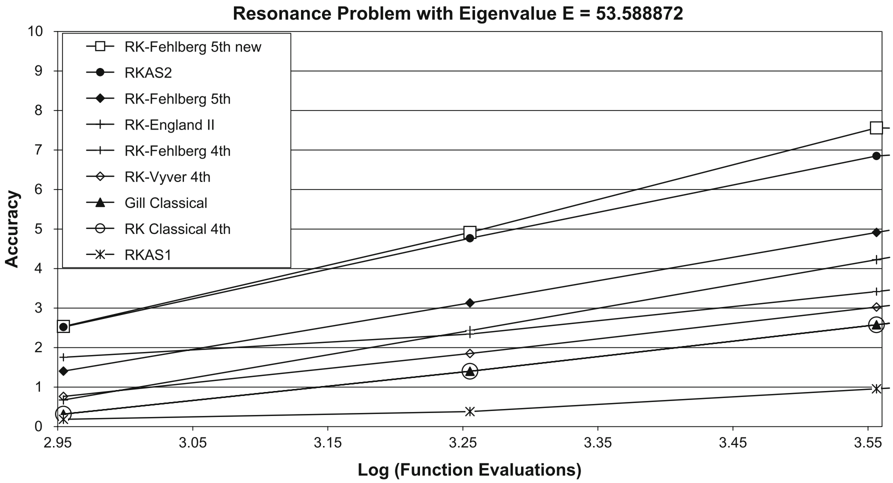

Fig. 1 Efficiency for the Schrödinger equation with $E = 53.588872$

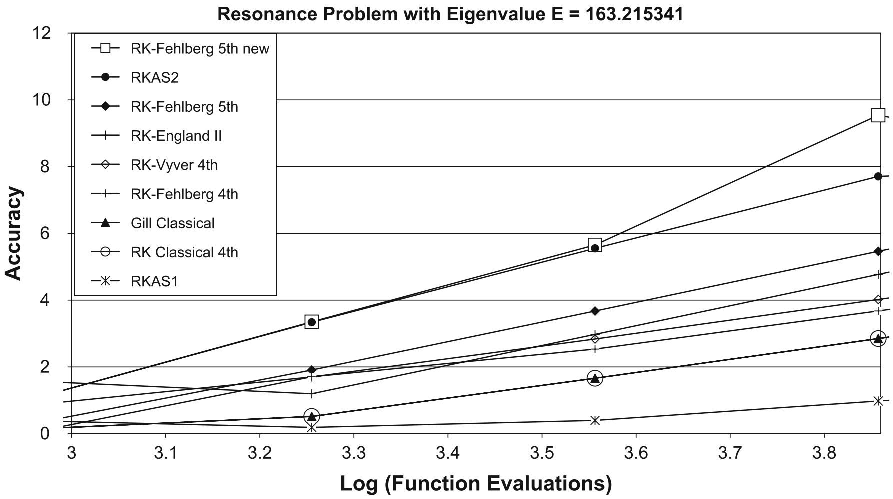

Fig. 2 Efficiency for the Schrödinger equation with $E = 163.215341$

4.1.3 Inhomogeneous problem

$$y'' = -100\,y + 99\,\sin(y)$$

with

$$\begin{aligned} y(0) &= 1 \\ y'(0) &= 11, \quad t \in [0,\ 1000\,\pi] \end{aligned} \tag{40}$$

Theoretical solution: $y(t) = \sin(t) + \sin(10\,t) + \cos(10\,t)$.

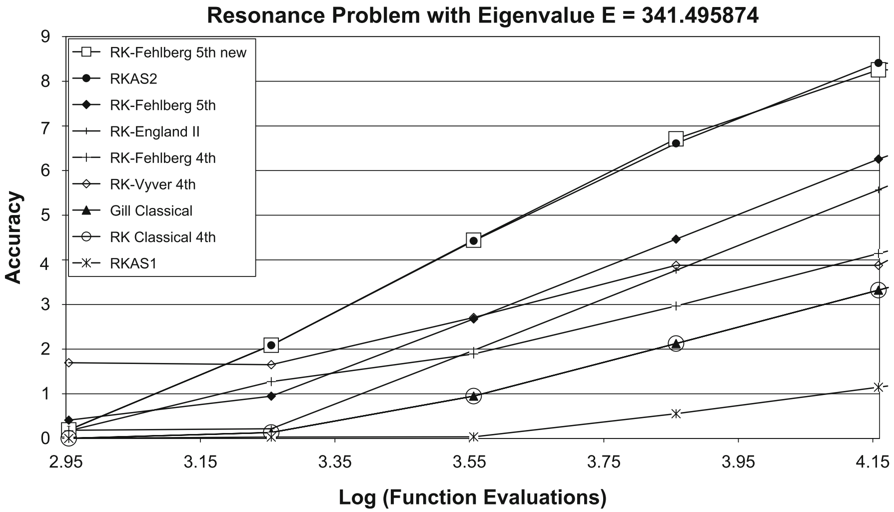

Fig. 3 Efficiency for the Schrödinger equation with $E = 341.495874$

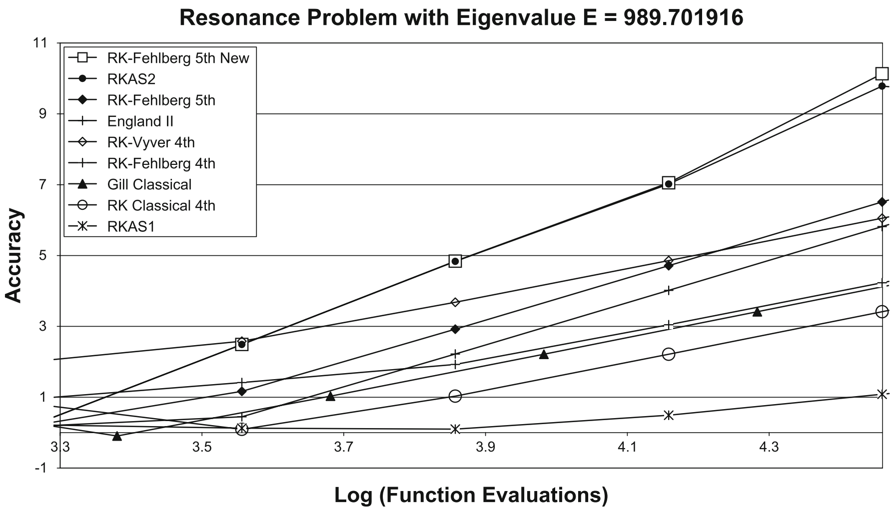

Fig. 4 Efficiency for the Schrödinger equation with $E = 989.701916$

4.1.4 *Duffing problem*

$$y'' = -y - y^3 + 0.002\ \cos(1.01\,t)$$

with

$$y(0) = 0.200426728067$$
$$y'(0) = 0, \qquad t \in [0,\ 1000\pi]$$

Theoretical solution: $y(t) = 0.200179477536 \cos(1.01\,t) + 2.46946143\,10^{-4} \cos(3.03\,t) + 3.04014\,10^{-7} \cos(5.05\,t) + 3.74\,10^{-10} \cos(7.07\,t) + \ldots$

4.2 The methods

In order to measure the efficiency of the method constructed in this paper we compare it to some already known methods, presenting the results of the best.

1. – **RK-Fehlberg 5th**: an explicit Runge-Kutta method with 6 stages and 5th algebraic order and 6th order of phase-lag [4].
   – **RK-Fehlberg 5th new**: a new explicit optimized Runge-Kutta method with 6 stages, 5th algebraic order constructed in this paper.

The following methods with 4th algebraic order have also been tested and they are presented:

2. – **Gill Classical method**: an explicit Runge-Kutta with 4 stages [4].
   – **Classical RK 4th**: the classical standard Runge-Kutta method [4].
   – **RK-Fehlberg 4th**: an explicit Runge-Kutta with 5 stages, 4th algebraic order and 4th order of phase-lag [4].
   – **RK-Vyver 4th**: an explicit, trigonometrically fitted Runge-Kutta method with 4 stages developed by Vyver [6].
   – **England II**: an explicit Runge-Kutta with 6 stages, 5th algebraic order and 6th order of phase-lag [4].
   – **RK-Franco**: an explicit Runge-Kutta with 6 stages and variable coefficients developed by Franco [5].
   – **RKAS1**: an explicit Runge-Kutta with 6 stages, 5th algebraic order and 6th phase-lag order developed by Anastassi and Simos [15].
   – **RKAS2**: an explicit Runge-Kutta with 6 stages, 5th algebraic order and 8th phase-lag order developed by Anastassi and Simos [15].

4.3 The Results

In Figs. 1, 2, 3 and 4 we present the efficiency of the methods for the Schrödinger equation for four different eigenenergies. We can notice that the new method, presented in this paper, **RK-Fehlberg 5th new**, has at least the same efficiency or higher than **RKAS2**,while has about two decimal digits higher accuracy than **RK-Fehlberg 5th**, which is the corresponding classical method of the new developed method. The latter has one digit higher accuracy than **England II**. Next in order of efficiency are **RK-Vyver 4th**, **Gill Classical**, **RK Classical 4th** and **RKAS1**.

In Fig. 5 we can see the efficiency of all the methods compared during the integration of the Nonlinear problem. We observe that the new method **RK-Fehlberg 5th new** is the most efficient of all other methods. Compared to the classical method **RK-Fehlberg 5th**, it has about two decimal digits higher accuracy. It is important to notice that the new method has at least the same efficiency or higher than **RKAS2** method and much more efficient from **RK-Franco** and **RK-Vyver 4th**, despite the fact that

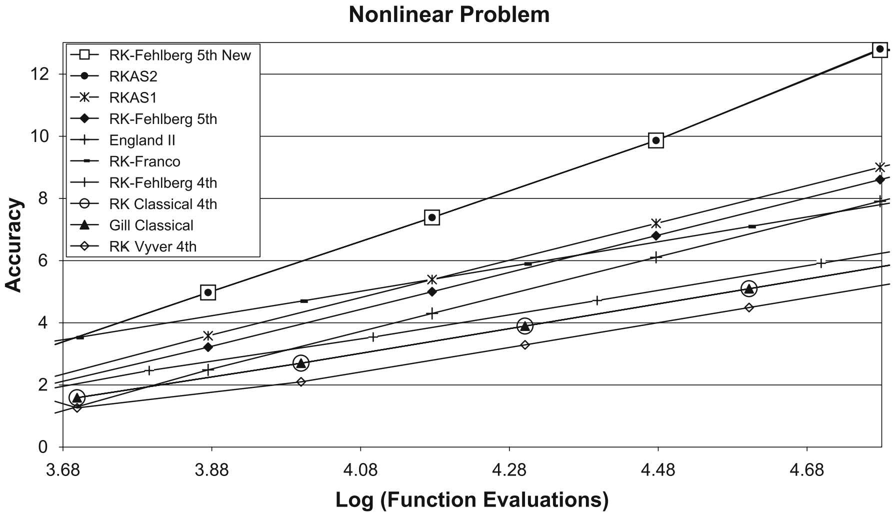

Fig. 5 Efficiency for the nonlinear problem

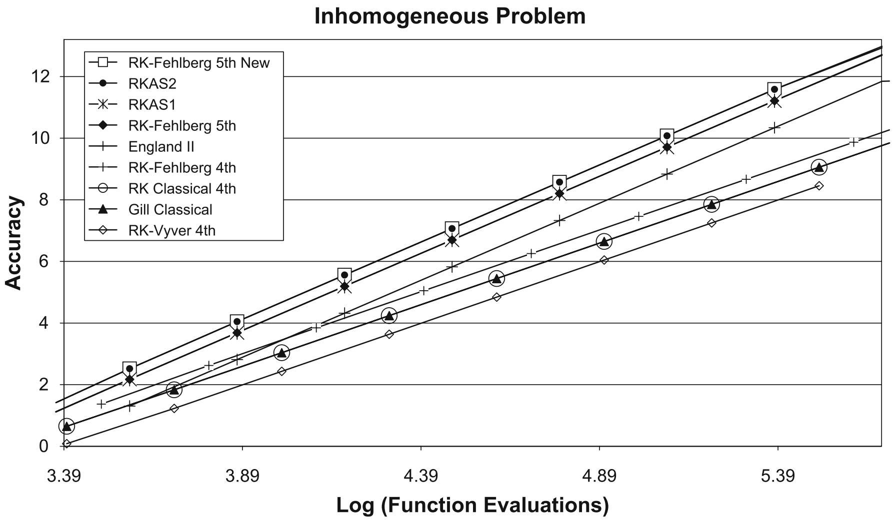

Fig. 6 Efficiency for the inhomogeneous problem

the latter methods have variable coefficients. In order of efficiency **RKAS1** method is third, next are **RK-Fehlberg 5th** and **England II**. **RK-Franco RK-Fehlberg 4th** follow, and last the **RK Classical 4th**, **Gill Classical**, and **RK-Vyver 4th**.

In Fig. 6 we can see the efficiency of the methods for the Inhomogeneous equation. We can see that **RK-Fehlberg 5th new**, is more efficient than **RK-Fehlberg 5th**, has at least the same efficiency with **RKAS2** and has about one decimal digit higher than **England II**, **RKAS1**, and **RK-Fehlberg 4th**, while the latter is also more efficient than **RK Classical 4th**, **Gill Classical**, and **RK-Vyver 4th**.

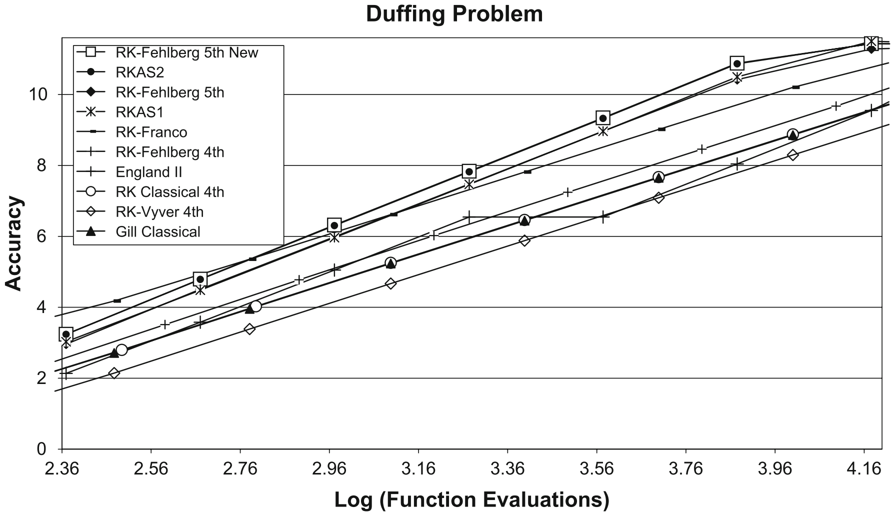

Fig. 7 Efficiency for the duffing problem

In Fig. 7 we can see the efficiency of the methods for the Duffing's equation. We can observe that the methods in descending order of efficiency are: **RK-Fehlberg 5th new**, **RKAS2**, **RK-Fehlberg 5th**, **RKAS1**, **RK-Franco**, **RK-Fehlberg 4th**, **England II**, **RK Classical 4th**, **RK-Vyver 4th**, **Gill Classical**.

5 Conclusions

A new optimized explicit Runge-Kutta Fehlberg method of fifth algebraic order is produced in this paper. This method is based on the Runge-Kutta Fehlberg method (27) and has increased order of phase-lag in comparison to the corresponding classical method, while the algebraic order is preserved. The results show the efficiency of the new constructed method, while it is compared to the corresponding classical method and other methods from the literature. It is remarkable that the Runge-Kutta Fehlberg 5th New is the most efficient in all problems tested, and particularly than the corresponding classical method: Runge-Kutta Fehlberg 5th method. This happens due to the optimization of the constant coefficients of the Runge-Kutta Fehlberg 5th method.

References

1. 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)
2. T.E. Simos, Ch. Tsitouras, A P-stable eighth order method for the numerical integration of periodic initial value problems. J. Comput. Phys. **130**, 123–128 (1997)
3. T.E. Simos, *Chemical Modelling—Applications and Theory Vol. 1, Specialist Periodical Reports* (The Royal Society of Chemistry, Cambridge, 2000), pp. 32–140
4. G. Engeln-Mullges, F. Uhlig, *Numerical Algorithms with Fortran* (Springer-Verlag, Berlin Heidelberg, 1996), pp. 423–488

5. J.M. Franco, Runge-Kutta methods adapted to the numerical integration of oscillatory problems. Appl. Numer. Math. **50**(3–4), 427–443 (2004)
6. H. Van de Vyver, Comparison of some special optimized fourth-order Runge-Kutta methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun., **166**, 109–122 (2005)
7. L. Aceto, A. Sestini, Numerical aspects of the coefficient computation for LMMs. J. Numer. Anal., Ind. Appl. Math. **3**, 181–191 (2008)
8. S. Chatterjee, M. Isaiay, F. Bonay, G. Badinoy, E. Venturino, Modelling environmental influences on wanderer spiders in the Langhe region (Piemonte-NW Italy). J. Numer. Anal., Ind. Appl. Math. **3**, 193–209 (2008)
9. C. Dagnino, V. Demichelis, P. Lamberti, A nodal spline collocation method for the solution of cauchy singular integral equations. J. Numer. Anal., Ind. Appl. Math. **3**, 211–220 (2008)
10. C. Enachescu, Approximation capabilities of neural networks. J. Numer. Anal., Ind. Appl. Math. **3**, 221–230 (2008)
11. O. Frederich, E. Wassen, F. Thiele, Prediction of the flow around a short wall-mounted finite cylinder using LES and DES. J. Numer. Anal., Ind. Appl. Math. **3**, 231–247 (2008)
12. H. Ogata, Fundamental solution method for periodic plane elasticity. J. Numer. Anal., Ind. Appl. Math. **3**, 249–267 (2008)
13. P.T. An, Some computational aspects of helly-type theorems. J. Numer. Anal., Ind. Appl. Math. **3**, 269–274 (2008)
14. A. Verhoeven, B. Tasic, T.G.J. Beelen, E.J.W. ter Maten, R.M.M. Mattheij, BDF compound-fast multirate transient analysis with adaptive stepsize control. J. Numer. Anal., Ind. Appl. Math. **3**, 275–297 (2008)
15. 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)
16. T.E. Simos, in *Atomic Structure Computations in Chemical Modelling: Applications and Theory*, ed. by A. Hinchliffe. UMIST, (The Royal Society of Chemistry, Cambridge, 2000), pp. 38–142
17. 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, Cambridge, 2002), pp. 170–270
18. 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)
19. 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)
20. 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)
21. 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)
22. 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)
23. 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)
24. 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)
25. 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)
26. 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)
27. T.E. Simos, Exponentially-fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
28. 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)
29. 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)

30. 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)
31. J. Vigo-Aguiar, 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)
32. 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)
33. 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)
34. 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 (2002)
35. 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)
36. 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)
37. 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)
38. 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)
39. 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)
40. 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)
41. 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)
42. 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)
43. 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)
44. 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)
45. 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)
46. T.E. Simos, G. Mousadis, Some new numerov-type methods with minimal phase-lag for the numerical-integration of the Radial Schrödinger-equation. Mol. Phys. **83**(6), 1145–1153 (1994)
47. T.E. Simos, A numerov-type method for the numerical-solution of the radial Schrödinger-equation. Appl. Numer. Math. **7**(2), 201–206 (1991)
48. G. Avdelas, T.E. Simos, Dissipative high phase-lag order numerov-type methods for the numerical solution of the Schrödinger equation. Phys. Rev. E **62**(1), 1375–1381 (2000)
49. T.E. Simos, P.S. Williams, Bessel and Neumann-fitted methods for the numerical solution of the radial Schrödinger equation. Comput. Chem. **21**(3), 175–179 (1997)