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# An Optimized Runge-Kutta-Nyström Method for the Numerical Solution of the Schrödinger Equation and Related Problems

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**Abstract**

In this paper, a new Runge-Kutta-Nyström method of fourth algebraic order is developed. The new method has zero phase-lag, zero amplification error and zero first derivatives of the previous properties. Numerical results indicate that the new method is much more efficient than other methods constructed for solving numerically the Schrödinger equation.

## 1 Introduction

In this paper we propose a new methodology, for deriving optimized methods, for the numerical integration of ordinary differential equations with oscillatory solutions. This type of ODEs often met in real problems, like the Schrödinger equation.

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In the recent past, many researchers developed methods with minimal phase-lag or phase lag of order infinity or a combination of those with zero dissipation. Such methods can be found in [2, 6, 8, 9, 12, 13, 15, 21, 22, 20].

Moreover several methods, based on phase, exponential or trigonometrically fitting, developed for solving numerically the Schrödinger equation (see [3, 4, 8, 9, 10, 11, 14, 16, 17, 18, 19, 23, 24, 25, 26, 28, 29, 30, 31]).

For the first time in the literature there is an attempt to combine the nullification of phase-lag and amplification factor with the nullification of their derivatives. The method that we are going to develop in this paper contains four variable coefficients, which depend on $v = \omega h$, where $\omega$ is the dominant frequency of the problem and $h$ is the step length of integration.

## 2 Phase lag and amplification error analysis of Runge-Kutta-Nyström methods

The initial value problem

$$\frac{d^2y(t)}{dt^2} = f(t, y(t)) \tag{1}$$

can be solved numerically by using Runge-Kutta-Nyström methods, which are of the form

$$\begin{aligned} y_n &= y_{n-1} + hy'_{n-1} + h^2 \sum_{i=1}^{m} b_i f(t_{n-1} + c_i h, f_i), \\ y_n &= y'_{n-1} + h \sum_{i=1}^{m} \hat{b}_i f(t_{n-1} + c_i h, f_i), \end{aligned} \tag{2}$$

where

$$f_i = y_{n-1} + hc_i y'_{n-1} + h^2 \sum_{j=1}^{i-1} \alpha_{ij} f(t_{n-1} + c_j h, f_j), \qquad i = 1, \ldots, m \tag{3}$$

more specifically for the explicit Runge-Kutta-Nyström methods $c_1 = 0$ and more specifically for an FSAL explicit RKN method $c_m = 1$ and $c_{m,j} = b_i$ for $j = i$.

By applying the RKN method (2) to the test equation

$$\frac{d^2y(t)}{dt^2} = (iw)^2 y(t) \Longrightarrow y''(t) = -w^2 y(t), \qquad \omega \in R \tag{4}$$

we obtain the numerical solution

$$\begin{bmatrix} y_n \\ hy'_n \end{bmatrix} = D^n \begin{bmatrix} y_0 \\ hy'_0 \end{bmatrix}, \quad D = \begin{bmatrix} A(z^2) & B(z^2) \\ \dot{A}(z^2) & \dot{B}(z^2) \end{bmatrix}, \quad z = \omega h, \tag{5}$$

where $A, B, \dot{A}, \dot{B}$ are polynomials in $z^2$, completely determined by the parameters of the method (2).

The eigenvalues of the amplification matrix $D$ are the roots of the characteristic equation

$$r^2 - tr(D)r + det(D) = 0 \tag{6}$$

In phase analysis one compares the phases of $exp(iz)$ with the phases of the roots of the characteristic equation (6). The following definition is originally formulated by van der Houwen and Sommeijer [2].

**Definition 1** *(Phase-lag). Apply the RKN method (2) to the general method (4). Then we define the phase-lag* $\Phi(z) = z - arccos(tr(D)/2\sqrt{det(D)})$. *If* $\Phi(z) = O(z^{q+1})$, *then the RKN method is said to have phase-lag order* $q$. *In addition, the quantity* $a(z) = 1 - \sqrt{det(D)}$ *is called amplification error.*

Let us denote

$$\begin{aligned} R(z^2) &= tr(D) = A(z^2) + \dot{B}(z^2) \\ Q(z^2) &= det(D) = A(z^2)\dot{B}(z^2) - \dot{A}(z^2)B(z^2) \end{aligned} \tag{7}$$

where $z = wh$. From definition 1 it follows that

$$\Phi(z) = z - arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right), \qquad a(z) = 1 - \sqrt{Q(z^2)}. \tag{8}$$

If at a point $z, a(z) = 0$, then the Runge-Kutta-Nyström method has zero dissipation at this point.

We can also put forward an alternative definition for the case of infinite order of phase lag.

**Definition 2** *(Phase-lag of order infinity). To obtain phase-lag of order infinity the relation* $\Phi(z) = z - arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = 0$ *must be hold.*

From definition 2 we have the following theorem.

**Theorem 1** If we have phase-lag of order infinity and at a point $z$, $\alpha(z) = 0$ then,

$$\left.\begin{array}{l} z - arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = 0 \\ 1 - \sqrt{Q(z^2)} = 0 \end{array}\right\} \Rightarrow \begin{array}{l} R(z^2) = 2cos(z) \\ Q(z^2) = 1 \end{array}$$

***Proof.***

$$\Phi(z) = z - arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = 0 \Leftrightarrow$$
$$arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = z \Leftrightarrow$$
$$cos\left(arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right)\right) = cos(z) \Leftrightarrow$$
$$\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = cos(z) \Leftrightarrow$$
$$\left(\frac{R(z^2)}{\sqrt{Q(z^2)}}\right) = 2cos(z). \tag{9}$$

Now for

$$a(z) = 0 \Leftrightarrow 1 - \sqrt{Q(z^2)} = 0 \Leftrightarrow \sqrt{Q(z^2)} = 1. \tag{10}$$

From the above relation and the expression (9) we have

$$R(z^2) = 2cos(z). \tag{11}$$

**Lemma 1** For the construction of a method with phase lag of order infinity and amplification error of order infinity, we must satisfy the conditions

$$R(z^2) = 2cos(z), Q(z^2) = 1$$

**Lemma 2** For the construction of a method with nullification of phase lag, amplification error and their derivatives, we must satisfy the conditions

$$R(z^2) = 2cos(z), Q(z^2) = 1, R'(z^2) = -2sin(z), Q'(z^2) = 0$$

# 3 Derivation of the new RKN method

In this part we present the derivation of the new algorithm, which is a four-stage explicit Runge-Kutta-Nyström method with the FSAL technique (first stage as last), so the method actually uses three stages at each step for the function evaluations. It is based on $R(z^2) = 2cos(z)$, $Q(z^2) = 1$, $R'(z^2) = -2sin(z)$, $Q'(z^2) = 0$ and on the following

coefficients that have been used by Dormand, El-Mikkawy and Prince in [1] :

$$\begin{aligned}
\alpha_{21} &= \frac{1}{32}, \qquad \alpha_{31} = \frac{7}{1000}, \qquad \alpha_{32} = \frac{119}{500}, \\
\alpha_{41} &= b_1, \qquad \alpha_{42} = b_2, \qquad \alpha_{43} = b_3 \\
c_2 &= \frac{1}{4}, \qquad c_3 = \frac{7}{10}, \qquad c_4 = 1, \\
b_1 &= \frac{1}{14}, \qquad b_2 = \frac{8}{27}, \qquad b_3 = \frac{25}{189}, \qquad b_4 = 0,
\end{aligned} \tag{12}$$

In order to evaluate the variable coefficients $\hat{b}_i$, $i = 1(1)4$, first we compute the polynomials $A, \dot{A}, B, \dot{B}$ in terms of RKN parameters. From these polynomials we obtain the expressions of $R(z^2)$ and $Q(z^2)$. Then we evaluate their derivatives $(R'(z^2), Q'(z^2))$. Through these calculations we lead to a system of four equations ($R(z^2) = 2cos(z)$, $Q(z^2) = 1$, $R'(z^2) = -2sin(z)$, $Q'(z^2) = 0$). Solving this system we obtain the coefficients $\hat{b}_i$, $i = 1(1)4$ , which are fully depended from the product $z$ of the step-length $h$ and the frequency $\omega$.

$$\begin{aligned}
\hat{b}_1 = -\frac{1}{252}\,(&62679\,z^{12} - 4328370\,z^{10} - 1956632\,z^9\sin(z) + 109558632\,z^8 \\
&-11739792\,z^8\cos(z) + 95584320\,z^7\sin(z) + 490636800\,z^6\cos(z) \\
&-1290787200\,z^6 - 1585664640\,z^5\sin(z) + 8157715200\,z^4 \\
&-6226156800\,z^4\cos(z) + 10911283200\,z^3\sin(z) + 29884723200\,z^2\cos(z) \\
&-29884723200\,z^2 - 24186470400\,z\sin(z) + 48372940800 \\
&-48372940800\,\cos(z))/ \\
&(z^4(289\,z^8 - 12240\,z^6 + 203040\,z^4 - 1555200\,z^2 + 4665600))
\end{aligned}$$

$$\begin{aligned}
\hat{b}_2 = \frac{2}{9}\,(&4373232\,z^8 - 483072\,z^8\cos(z) - 80512\,z^9\sin(z) + 2040422400 \\
&+389145600\,z^3\sin(z) - 54777600\,z^5\sin(z) + 3429440\,z^7\sin(z) - \\
&1020211200\,z\sin(z) - 1118361600\,z^2 + 308021760\,z^4 + 17166720\,z^6\cos(z) \\
&-214709760\,z^4\cos(z) + 1118361600\,z^2\cos(z) - 193800\,z^{10} + 3315\,z^{12} \\
&-2040422400\,\cos(z) - 49307520\,z^6) \\
&/(z^4(289\,z^8 - 12240\,z^6 + 203040\,z^4 - 1555200\,z^2 + 4665600))
\end{aligned}$$

$$\hat{b}_3 = -\frac{125}{63}\,(211248\,z^8 - 14688\,z^8\cos(z) - 2448\,z^9\sin(z) + 36218880\,z^3\sin(z) - 3870720\,z^5\sin(z) + 173696\,z^7\sin(z) + 248832000 - 124416000\,z\sin(z) - 113909760\,z^2 + 26150400\,z^4 + 938496\,z^6\cos(z) - 16819200\,z^4\cos(z) + 113909760\,z^2\cos(z) - 5916\,z^{10} + 51\,z^{12} - 248832000\,\cos(z) - 3297216\,z^6)$$
$$/(z^4(289\,z^8 - 12240\,z^6 + 203040\,z^4 - 1555200\,z^2 + 4665600))$$

$$\hat{b}_4 = -(1/8)\,(289\,z^{12} - 192153600\,z^3\sin(z) - 619315200\,z^2\cos(z) - 12240\,z^{10} - 22320\,z^8 + 1857945600\,\cos(z) - 293760\,z^7\sin(z) - 1857945600 - 1175040\,z^6\cos(z) + 6877440\,z^6 + 13532160\,z^5\sin(z) - 99855360\,z^4 + 56309760\,z^4\cos(z) + 619315200\,z^2 + 928972800\,z\sin(z))$$
$$/(z^4(289\,z^8 - 12240\,z^6 + 203040\,z^4 - 1555200\,z^2 + 4665600))$$

For small values of $x$ the following Taylor series expansions are used

$\hat{b}_1 = \frac{1}{14} + \frac{163}{22680}\,z^2 - \frac{979}{169344}\,z^4 - \frac{233483}{587865600}\,z^6 - \frac{2318623}{67898476800}\,z^8 - \frac{6628679977}{4448708199936000}\,z^{10}$

$\hat{b}_2 = \frac{32}{81} - \frac{14}{405}\,z^2 + \frac{13837}{1837080}\,z^4 + \frac{18353}{55112400}\,z^6 + \frac{1458319}{43649020800}\,z^8 + \frac{20065057}{11916182678400}\,z^{10}$

$\hat{b}_3 = \frac{250}{567} + \frac{425}{6804}\,z^2 - \frac{7915}{5143824}\,z^4 - \frac{1805}{8817984}\,z^6 - \frac{984869}{24443451648}\,z^8 - \frac{128490611}{26692249199616}\,z^{10}$

$\hat{b}_4 = \frac{5}{54} - \frac{341}{9720}\,z^2 - \frac{97}{51840}\,z^4 - \frac{2147}{18370800}\,z^6 + \frac{7697}{2217093120}\,z^8 + \frac{30952913}{15131660544000}\,z^{10}$

# 4 Numerical results

## 4.1 Schrödinger equation

The one-dimensional or radial time-independent Schrödinger equation has the form

$$y''(x) + \left(E - \frac{l(l+1)}{x^2} - V(x)\right)y(x) = 0, \qquad where \quad 0 \le x < \infty \tag{13}$$

We call the term $l(l+1)/x^2$ the *centrifugal potential*, and the function $V(x)$ the *electric potential*. In (13), $E$ is a real number denoting the *energy*, and $l$ is a *quantum number*. The function $W(x) = l(l+1)/x^2 + V(x)$ denotes the *effective potential*, where $\lim_{x\to\infty} V(x) = 0$ and so $\lim_{x\to\infty} W(x) = 0$. The boundary condition are $y(0) = 0$ together with a second boundary condition, for large values of x, determined by the physical considerations.

### 4.1.1 Resonance problem

For the purpose of our numerical illustration we will take the domain of integration as $x \in [0, 15]$, using the Woods-Saxon potential:

$$V(x) = \frac{u_0}{1+q} + \frac{u_1 q}{(1+q)^2}, \qquad q = exp\left(\frac{x - x_0}{\alpha}\right), \quad where \tag{14}$$
$$u_0 = -50, \quad \alpha = 0.6, \quad x_0 = 7, \quad u_1 = -\frac{u_0}{\alpha}$$

In the case of positive energies ($E = k^2$), the potential ($V(x)$) dies away faster than the centrifugal potential ($l(l+1)/x^2$), so for a large number for $x$, Schrödinger equation effectively reduces to

$$y''(x) + (k^2 - \frac{l(l+1)}{x^2})y(x) = 0 \tag{15}$$

The above equation (15) has two linearly independent solutions, $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l$ and $n_l$ are the spherical Bessel and Neumann functions, respectively. When $x \to \infty$, the solution of equation (13) take the following asymptotic form

$$y(x) \simeq Akxj_l(kx) - Bkxn_l(kx)$$
$$\simeq D\left[sin\left(kx - \frac{l\pi}{2}\right) + tan(\delta_l)cos\left(kx - \frac{l\pi}{2}\right)\right], \tag{16}$$

where $\delta_l$ is the scattering phase shift that may be calculated from the bellow formula

$$tan(\delta_l) = \frac{y(x_i)S(x_{i+1}) - y(x_{i+1})S(x_i)}{y(x_{i+1})C(x_i) - y(x_i)C(x_{i+1})}, \tag{17}$$

where $S(x) = kxj_l(kx), \quad C(x) = kxn_l(kx)$ and $x_i < x_{i+1}$ both exist in the asymptotic region.

For positive energies and for $l = 0$, we calculate the phase shift ($\delta_l$) and then we compare it with the accurate value which is $\pi/2$. The boundary conditions for this eigenvalue problem are $y(0) = 0$ and $y(x) = cos(\sqrt{E}x)$ for large x.

We use the following eigenenergies

$E_1 = 53.588872$

$E_2 = 163.215341$

$E_3 = 341.495874$

$E_4 = 989.701916$

We also consider the case where $l \neq 0$. Specifically we use the Lennard-Jones potential given by the formula $V(x) = m\left(\frac{1}{x^{12}} - \frac{1}{x^6}\right)$, where $m = 500$, for $l = \{0, 1, 2, \ldots, 10\}$, $E = \{25, 100\}$ and step-length of integration $h = 0.1$. We compare the phase-shifts with the values found at [27] and present the decimal digits that the approximate solutions agree with the reference solution. The results are given in the two tables of subsection 4.3.

#### 4.1.2 Bound-states problem

In the case of negative energies ($E < 0$), we consider the eigenvalue problem with boundary conditions

$y(0) = 0$ and $y(x) = exp(-\sqrt{-E}x)$ for large x.

In order to solve this problem numerically, by a chosen eigenvalue, we integrate forward from the point $x = 0$, backward from the point $x = 15$ and matching up the solution at some internal point in the range of integration.

For the Bound-states problem we use the following eigenenergies

$E_1 = -49.457788728$

$E_2 = -41.232607772$

$E_3 = -26.873448915$

$E_4 = -8.676081670$

The frequency is given by the suggestion of Ixaru and Rizea [4]

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

### 4.2 Nonlinear problem

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

### 4.3 Comparison

We are going to compare our results to those derived by using the high order method of embedded Runge-Kutta-Nyström 4(3)4 method, of *DEP* (see [1]), as well as to other methods derived for the numerical solution of second order differential equations. The methods used in the comparison have been denoted by:

• DPAFRKN4: The new fourth-order RKN method with four stages (three effective stases with FSAL property), derived in Section 3.

• RKN4: The high order method of pair RKN 4(3)4 method of *Dormand, El-Mikkawy and Prince* with four stages (three effective stases with FSAL property)[1].

• VDVEFRKN4: The fourth-order RKN method with four stages (three effective stases with FSAL property), derived by *Vyver* [7] (Section 3.1).

• FREFRKN4: The exponentially fitted, fourth-order RKN method with four stages (three effective stases with FSAL property), derived by *Franco* [5] (Section 3.3).

One way to measure the efficiency of the method is to compute the accuracy in the decimal digits, that is $-log_{10}(error\ at\ the\ end\ point)$ when comparing the phase shift to the actual value $\pi/2$ versus the computational effort measured by the $log_{10}(number\ of\ function\ evaluations\ required)$. In the figures we display the efficiency curves, that is the accuracy versus the computational cost measured by the number of function evaluations required by each method.

| $l$ (E=25) | *Kobeissi et al.* | *NEW* | *FREF* | *RKN4* | *VDVEF* |
|---|---|---|---|---|---|
| 0 | −0.48302543 | 2.13 | 1.74 | 1.88 | 1.75 |
| 1 | 0.92824634 | 2.14 | 1.75 | 1.89 | 1.75 |
| 2 | −0.96354014 | 2.17 | 1.77 | 1.91 | 1.77 |
| 3 | 0.12073704 | 2.20 | 1.79 | 1.93 | 1.79 |
| 4 | 1.03290370 | 2.25 | 1.82 | 1.97 | 1.82 |
| 5 | −1.37840550 | 2.31 | 1.85 | 2.01 | 1.86 |
| 6 | −0.84398975 | 2.39 | 1.90 | 2.07 | 1.90 |
| 7 | −0.52543971 | 2.48 | 1.95 | 2.13 | 1.95 |
| 8 | −0.45743790 | 2.57 | 2.00 | 2.19 | 2.00 |
| 9 | −0.75702397 | 2.65 | 2.05 | 2.26 | 2.05 |
| 10 | 1.41486080 | 2.96 | 2.17 | 2.42 | 2.18 |

| $l$ (E=100) | *Kobeissi et al.* | *NEW* | *FREF* | *RKN4* | *VDVEF* |
|---|---|---|---|---|---|
| 0 | −0.43100436 | 1.92 | 0.60 | 0.88 | 0.62 |
| 1 | 1.04500840 | 1.93 | 0.61 | 0.88 | 0.62 |
| 2 | −0.71580773 | 1.95 | 0.61 | 0.88 | 0.62 |
| 3 | 0.56880667 | 1.98 | 0.61 | 0.89 | 0.63 |
| 4 | −1.38576670 | 2.02 | −0.46 | 0.90 | −0.46 |
| 5 | −0.29834254 | 2.07 | 0.62 | 0.90 | 0.64 |
| 6 | 0.68682901 | 2.13 | 0.63 | 0.92 | 0.65 |
| 7 | 1.56630270 | 2.20 | 0.64 | 0.93 | 0.66 |
| 8 | −0.80594020 | 2.28 | 0.66 | 0.95 | 0.67 |
| 9 | −0.15240790 | 2.36 | 0.67 | 0.96 | 0.68 |
| 10 | 0.37789982 | 2.44 | 0.68 | 0.98 | 0.69 |

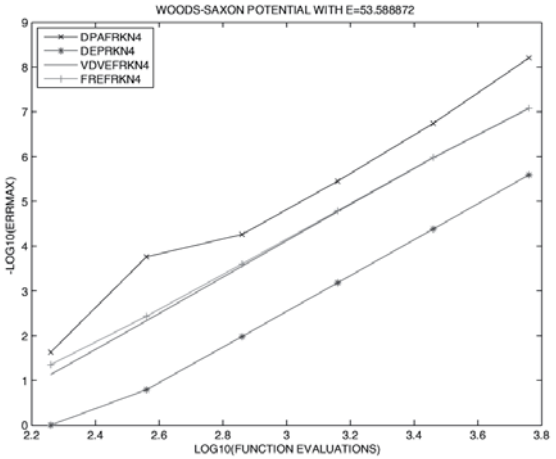


Figure 1: Efficiency for the Schrödinger equation using E=53.588872

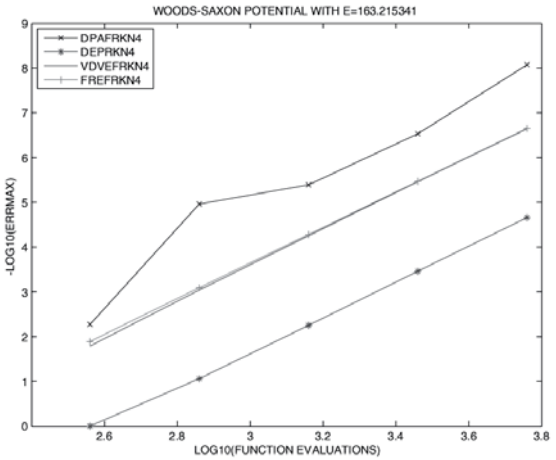


Figure 2: Efficiency for the Schrödinger equation using E=163.215341

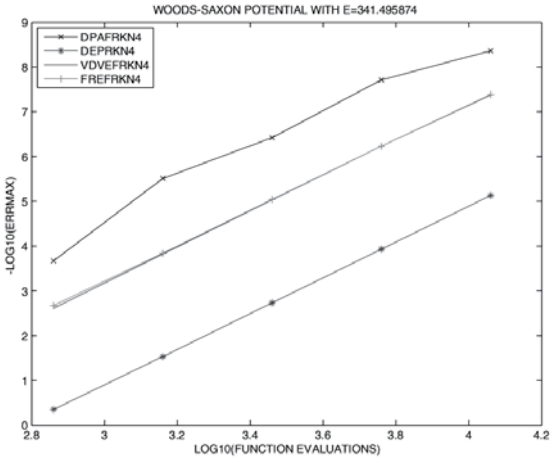


Figure 3: Efficiency for the Schrödinger equation using E=341.495874

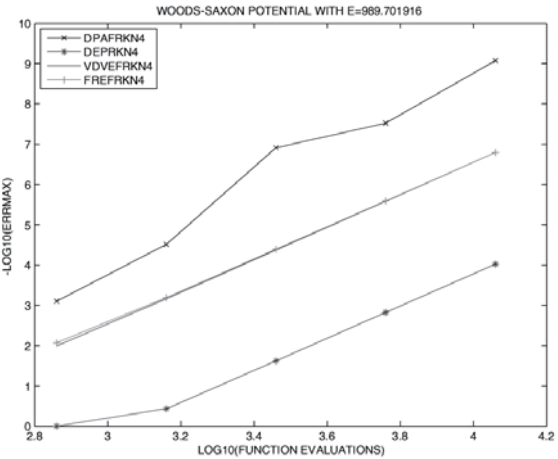


Figure 4: Efficiency for the Schrödinger equation using E=989.701916

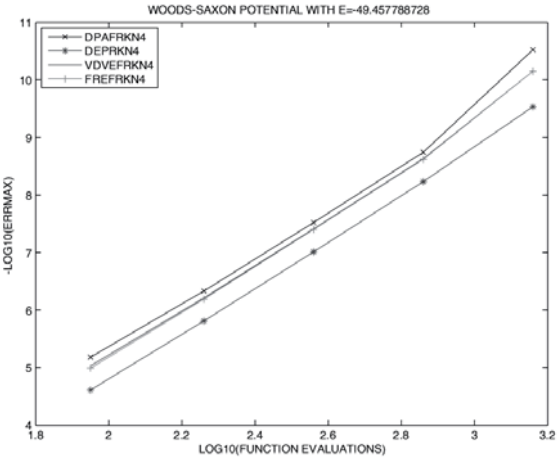


Figure 5: Efficiency for the Schrödinger equation using E=-49.457788728

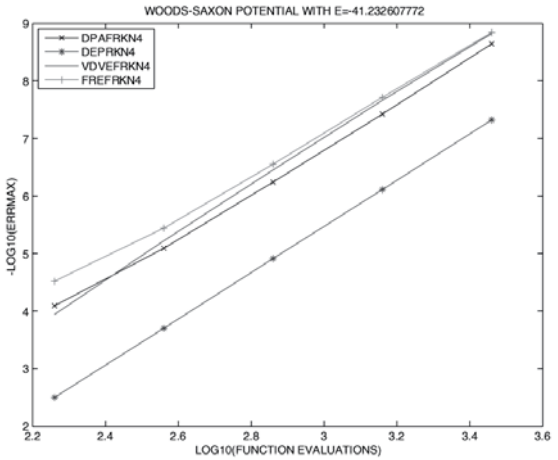


Figure 6: Efficiency for the Schrödinger equation using E=-41.232607772

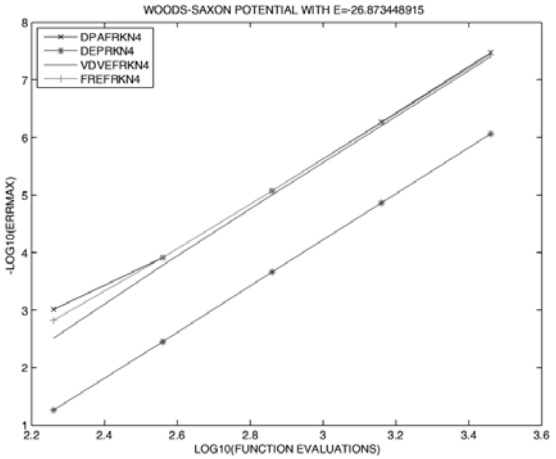


Figure 7: Efficiency for the Schrödinger equation using E=-26.873448915

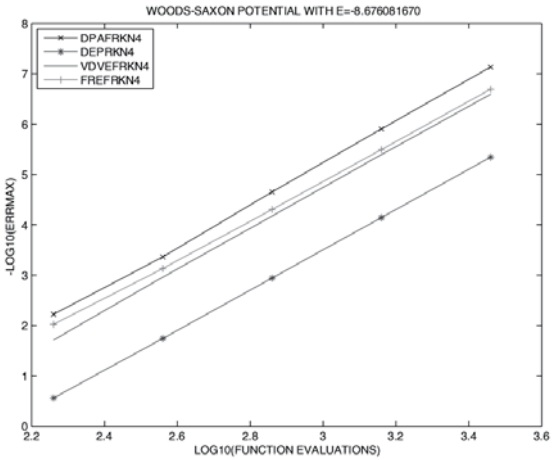


Figure 8: Efficiency for the Schrödinger equation using E=-8.676081670

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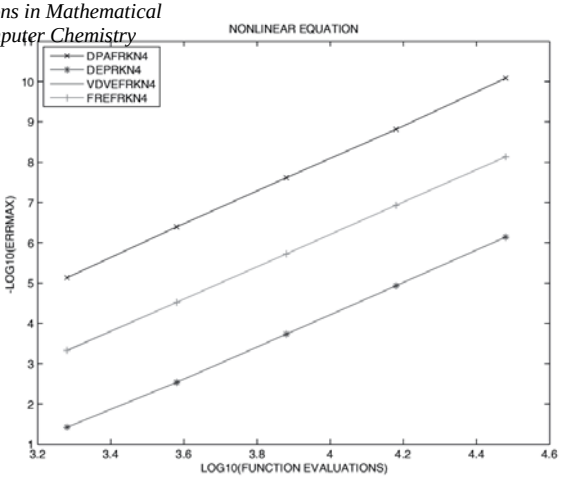


Figure 9: Efficiency for the Nonlinear equation

## 5 Conclusions

The optimized RKN method, derived in this paper is much more efficient than the classical one in all cases. Moreover, we observe that for the bound-states problem the three methods (DPAFRKN4, VDVEFRKN4 and FREFRKN4) achieved almost the same accuracy. When integrating the resonance problem and the nonlinear equation, the numerical results show the superiority of the new technique.

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