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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 *

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The generator of tenth-order hybrid explicit methods, the basic method of which has been developed in part 1, is constructed and also optimized, by maximization of the intervals of periodicity. The efficiency of the new methods is shown by their application to the coupled differential equations of the Schrödinger type.

KEY WORDS: phase-lag, hybrid methods, explicit methods, algebraic order, intervals of stability, Schrödinger equation, periodic problems, initial-value problems

1. Introduction

Researchers in numerous topics in scientific areas, such as theoretical physics, quantum mechanics, atomic physics, molecular physics, theoretical chemistry, astrophysics, chemical physics, electronics and elsewhere (see [1,2]) show a lot of interest for the solution of special second order periodic initial-value problems of the form:

$$y'' = f(x, y), \qquad y(x_0) = y_0, \quad y'(x_0) = y'_0. \tag{1}$$

Lately great activity has been observed [3–18,27] for the numerical solution of problems of the form equation (1). Some of the characteristics of the numerical methods, used in the solution of the above problems are the maximum algebraic order, the maximum phase-lag order and the maximum interval of periodicity.

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In paper [19] the development of the basic method of a generator of hybrid explicit methods for the numerical solution of the Schrödinger equation is described. The methods are of tenth algebraic order. In this paper we create the generator, and the analysis of the optimization of the generator is given. We call generator, a family of methods, in which the coefficients of the methods are defined *automatically*. This is very important for error-control procedures, since we can use, without computational cost, all the methods of the family, in order to increase the step-size of integration. The methods have minimal phase-lag. The coefficients of the methods of the generator are calculated appropriately, in order to satisfy this property.

In section 2 the analysis of the phase-lag for symmetric two-step methods is presented. The derivation of the methods' parameters is given in section 3. In the next section the construction of the optimized generator is explained. Stability analysis is shown in section 5. In section 6 an automatic error control mechanism is given and a variable step procedure, which is based on the new methods, is described. Finally, numerical results and comparison of the generators with some other methods are illustrated.

2. Phase-lag analysis

Based on Lambert and Watson [4], we use the scalar test equation

$$y'' = -w^2 y, \tag{2}$$

in order to investigate the stability properties of methods for solving the initial-value problem equation (1) and the interval of periodicity.

When we apply a symmetric two-step method to the scalar equation (2), we obtain a difference equation of the form:

$$y_{n+1} - 2C(s)y_n + y_{n-1} = 0, \tag{3}$$

where $s = wh$, h is the step length, $C(s) = B(s)/A(s)$, where $A(s)$ and $B(s)$ are polynomials in s, and y_n is the computed approximation to $y(nh)$, $n = 0, 1, 2, \ldots$.

The characteristic equation associated with (3) is

$$z^2 - 2C(s)z + 1 = 0. \tag{4}$$

Bruca and Nigro [5] introduced the frequency distortion as an important property of a method for solving special second order initial-value problems. For frequency distortion, other authors use the terms of *phase-lag, phase-error* or *dispersion*. From now on, we use the term *phase-lag*.

The roots of the characteristic equation (4) are denoted as z_1 and z_2.

We have the following definitions:

Definition 1 [10,11,17,20]. The method (3) is unconditionally stable if $|z_1| \leqslant 1$ and $|z_2| \leqslant 1$ for all values of s.

Definition 2. Following Lambert and Watson [4], we say that the numerical method equation (3) has an interval of periodicity $(0, s_0^2)$, if for all $s^2 \in (0, s_0^2)$, z_1 and z_2 satisfy

$$z_1 = \mathrm{e}^{\mathrm{i}\beta(s)} \quad \text{and} \quad z_2 = \mathrm{e}^{-\mathrm{i}\beta(s)}, \tag{5}$$

where $\beta(s)$ is a real function of s. For any method corresponding to the characteristic equation (4), the phase-lag is defined as the leading term in the expansion of

$$t = s - \beta(s) = s - \cos^{-1}\bigl[C(s)\bigr]. \tag{6}$$

If the quantity $t = \mathrm{O}(s^{q+1})$ as $s \to 0$, the order of phase-lag is q.

Definition 3 [6]. The method (3) is *P-stable* if its *interval of periodicity* is $(0, \infty)$.

Theorem 1. A method, which has the characteristic equation (4) has an interval of periodicity $(0, s_0^2)$, if for all $s^2 \in (0, s_0^2)$ $|C(s)| < 1$.

Theorem 2. About the method, which has an interval of periodicity $(0, s_0^2)$, we can write:

$$\cos\bigl[\beta(s)\bigr] = C(s), \quad \text{where } s^2 \in \bigl(0, s_0^2\bigr). \tag{7}$$

For the proofs of the above theorems see [18].

We note that van der Houwen and Sommeijer [20] and Coleman [10] have chosen this approach to find the phase-lag. Based on this, Coleman [10] arrived at the following remark.

Remark 1. If the phase-lag order is $q = 2r$, then we have:

$$\begin{aligned} &t = cs^{2r+1} + \mathrm{O}\bigl(s^{2r+3}\bigr) \\ &\quad \Longrightarrow \quad \cos(s) - C(s) = \cos(s) - \cos(s - t) = cs^{2r+2} + \mathrm{O}\bigl(s^{2r+4}\bigr). \end{aligned} \tag{8}$$

With the properties of the *interval of periodicity* and the *phase-lag*, it is easy to see why the Numerov's method is so popular for the numerical solution of problems of the form (1), since it has a larger interval of periodicity than the sixth-order four-step methods and has the same phase-lag order (four) compared with the four-step methods.

3. Derivation of the free parameters w_i of the generator

Theorem 3. Application of the family of methods introduced in [19] to the scalar test equation (2) leads to the difference equation (3) with $A(s) = 1$ and $B(s)$ given by:

$$\begin{aligned} B(s) = {} & \sum_{i=0}^{5} (-1)^i \frac{1}{(2i)!} s^{2i} - \frac{112943657}{152374763520000} s^{12} - \frac{122489653693}{1645647446016000000} s^{14} \\ & - \frac{30495677389}{19747769352192000000} s^{16} - \frac{93281051}{13165179568128000000} s^{18} \end{aligned}$$

$$+\big(\tfrac{17081263}{2^{20}3^{11}5^{2}}+\tfrac{73363119059}{2^{23}3^{14}5^{4}7}s^{2}+\tfrac{16305968459}{2^{24}3^{15}5^{4}7}s^{4} + \tfrac{4596390901}{2^{27}3^{16}5^{5}}s^{6}+\tfrac{93281051}{2^{28}3^{15}5^{5}7}s^{8}\big)\sum_{i=6}^{b+6}\Bigg[(-1)^{i+1}s^{2i}2^{i}\prod_{j=b}^{b+6-i}w_j\Bigg], \tag{9}$$

where b denotes each method of the family and is defined by the user. The proof is given in appendix.

Our methods are explicit, so it is obvious that $C(s)=B(s)$.

In order to facilitate our work, we call AR and AT the quantities given below:

$$AR=\big(\tfrac{17081263}{2^{20}3^{11}5^{2}}s^{12}+\tfrac{73363119059}{2^{23}3^{14}5^{4}7}s^{14}+\tfrac{16305968459}{2^{24}3^{15}5^{4}7}s^{16}+\tfrac{4596390901}{2^{27}3^{16}5^{5}}s^{18}+\tfrac{93281051}{2^{28}3^{15}5^{5}7}s^{20}\big), \tag{10}$$

$$AT=\sum_{i=6}^{b+6}\Bigg[(-1)^{i+1}s^{2i-12}2^{i}\prod_{j=b}^{b+6-i}w_j\Bigg]. \tag{11}$$

We calculate the phase-lag.

$$\begin{aligned}\frac{1}{s^2}\big[\cos(s)-B(s)\big]&=\frac{1}{s^2}\Bigg[\sum_{i=0}^{\infty}(-1)^{i}\tfrac{1}{(2i)!}s^{2i}-\sum_{i=0}^{5}(-1)^{i}\tfrac{1}{(2i)!}s^{2i}+\tfrac{112943657}{152374763520000}s^{12}\\&\quad+\tfrac{122489653693}{1645647446016000000}s^{14}+\tfrac{30495677389}{19747769352192000000}s^{16}\\&\quad+\tfrac{93281051}{1316517956812800000}s^{18}-AR\cdot AT\Bigg]\\&=\frac{1}{s^2}\Bigg[\sum_{i=6}^{\infty}(-1)^{i}\tfrac{1}{(2i)!}s^{2i}+\tfrac{112943657}{152374763520000}s^{12}\\&\quad+\tfrac{122489653693}{1645647446016000000}s^{14}+\tfrac{30495677389}{19747769352192000000}s^{16}\\&\quad+\tfrac{93281051}{1316517956812800000}s^{18}-AR\cdot AT\Bigg],\end{aligned} \tag{12}$$

$$\begin{aligned}&\frac{1}{s^2}\big[\cos(s)-B(s)\big]=0\\&\implies\quad\frac{1}{s^2}\Big[\tfrac{1}{12!}s^{12}-\tfrac{1}{14!}s^{14}+\tfrac{1}{16!}s^{16}-\tfrac{1}{18!}s^{18}+\tfrac{112943657}{152374763520000}s^{12}\\&\qquad+\tfrac{122489653693}{1645647446016000000}s^{14}+\tfrac{30495677389}{19747769352192000000}s^{16}\\&\qquad+\tfrac{93281051}{1316517956812800000}s^{18}-AR\cdot AT\Big]=0\\&\implies\quad\frac{1}{s^2}\Big[\tfrac{1245879427}{1676122398720000}s^{12}+\tfrac{122593247666693}{1647293093462016000000}s^{14}+\tfrac{30527117850389}{1976751712154419200000}s^{16}\\&\qquad+\tfrac{1587328652867}{2240318607108341760000000}s^{18}-AR\cdot AT\Big]=0\end{aligned}$$

$$
\begin{aligned}
\Longrightarrow \quad & \tfrac{1245879427}{1676122398720000}s^{10} + \tfrac{122593247666693}{1647293093462016000000}s^{12} \\
& \quad + \tfrac{30527117850389}{1976751712154419200000}s^{14} + \tfrac{1587328652867}{2240318607108341760000000}s^{16} \\
& \quad = \Big(\tfrac{17081263}{2^{20}3^{11}5^{2}}s^{10} + \tfrac{73363119059}{2^{23}3^{14}5^{4}7}s^{12} + \tfrac{16305968459}{2^{24}3^{15}5^{4}7}s^{14} \\
& \quad + \tfrac{4596390901}{2^{27}3^{16}5^{5}}s^{16} + \tfrac{93281051}{2^{28}3^{15}5^{5}7}s^{18}\Big) \sum_{i=6}^{b+6}\left[(-1)^{i+1}s^{2i-12}2^{i}\prod_{j=b}^{b+6-i} w_j\right] \\
\Longrightarrow \quad & \sum_{i=6}^{b+6}\left[(-1)^{i+1}s^{2i-12}2^{i}\prod_{j=b}^{b+6-i} w_j\right] = u_0 + u_1 s^2 + u_2 s^4 + \cdots \\
\Longrightarrow \quad & -2^6 w_b + 2^7 s^2 w_b w_{b-1} + \cdots + (-1)^{b+7}2^{b+6}s^{2(b+6)-12}w_b w_{b-1}\cdots w_0 \\
& \quad = u_0 + u_1 s^2 + u_2 s^4 + \cdots. \qquad (13)
\end{aligned}
$$

The formula obtained for w_i is:

$$
w_{b-i} = (-1)^{i+1}\frac{u_i}{2^{i+6}\prod_{j=b}^{b-i+1} w_j}, \qquad (14)
$$

where $i = 0, 1, \ldots, b$ and $\prod_{j=b}^{b-i+1} w_j = 1$ for $i = 0$.

We clarify the formula (14), with an example.

According to the desired approximation, we choose the value of b. For $b = 5$, using formula (14) we obtain:

$$
w_5 = -\frac{u_0}{2^6}, \qquad w_4 = \frac{u_1}{2^7 w_5}, \qquad w_3 = -\frac{u_2}{2^8 w_5 w_4}, \qquad w_2 = \frac{u_3}{2^9 w_5 w_4 w_3},
$$
$$
w_1 = -\frac{u_4}{2^{10} w_5 w_4 w_3 w_2}, \qquad w_0 = \frac{u_5}{2^{11} w_5 w_4 w_3 w_2 w_1}.
$$

4. Optimized generator

Based on the generator of methods presented previously, we intent to construct another one with better stability. In order to accomplish this, we work as follows. For every method of the family we maintain the parameter w_0 free. Applying the formulae (9) and (14), $i = 0, \ldots, b-1$, we find the values of $B(s)$ and w_j, $j = b(-1)1$, and using maximization techniques, we calculate with efficient approximation the parameter w_0, trying to obtain larger intervals of periodicity.

5. Stability analysis

According to theorem 1, it follows that a symmetric two step method has a non-empty interval of periodicity, if $A(s) \pm B(s) > 0$ for all s^2 in $(0, s_0^2)$. Based on the fact, that the methods we produce are explicit, we have $A(s) = 1$.

Table 1
Intervals of periodicity for several methods of the generator.

b	Int. of period.	b	Int. of period.
0	12.62	1	16.22
2	8.66	3	14.02
4	9.02	5	14.40
6	9.30	7	14.63
8	9.48	9	14.76
$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 2
Intervals of periodicity for several methods after the optimization of the generator.

b	Int. of period.	b	Int. of period.
0	14.39	1	20.16
2	21.68	3	15.90
4	20.24	5	16.01
6	19.92	7	16.05
8	14.63	9	16.03
$\vdots$	$\vdots$	$\vdots$	$\vdots$

In order to find the stabilities of the new generators, we calculate $B(s)$, equation (9). The intervals of periodicity for some methods of the first generator, are given in table 1 and for some methods of the optimized generator, are given in table 2. In tables 1 and 2, b denotes the method of the family and is chosen according to the will of the user.

6. Application of the new method. Comparison of the results

We apply the new family of explicit methods, the optimized one and the eighth algebraic order Runge–Kutta–Nyström method of Dormand et al. [21] to the coupled differential equations of the Schrödinger type and we compare the results extracted. For every point x between the boundaries, we have set, we obtain the absolute difference between the numerical and the theoretical solution of the problem. We call the maximum of these differences *the absolute error*.

6.1. Local error estimation

In order to estimate the local truncation error (LTE) for the integration of systems of initial-value problems, many methods are used in the literature (see, for example, [12–15,22] and references therein).

In this paper the local error estimation technique is based on an embedded pair of integration methods and on the fact that, when the phase-lag order is maximal, then the approximation of the solution for problems with an oscillatory or periodic solution is better.

We have the following definition.

Definition 4. We define the *local phase-lag* error estimate in the lower order solution y^L_{n+1} by the quantity

$$E_{\mathrm{pl}} = \left| y^H_{n+1} - y^L_{n+1} \right|, \tag{15}$$

where y^H_{n+1} is the solution obtained with higher phase-lag order method and y^L_{n+1} is the solution obtained with lower phase-lag order method. In the present case y^H_{n+1} is the solution obtained using the b family of methods, while y^L_{n+1} is the solution obtained using the $b-1$ family of methods developed in sections 3 and 4. Under the assumption that h is sufficiently small, the *local error* in y^H_{n+1} can be neglected compared with that in y^L_{n+1}.

If a local error of *TOL* is requested and the nth step of the integration procedure is obtained using a step size equal to h_n, the estimated step size for the $(n+1)$st step, which would give a local error of *TOL*, must be

$$h_{n+1} = h_n \left(\frac{TOL}{E_{\mathrm{pl}}} \right)^{1/q}, \tag{16}$$

where q is the phase-lag order of the method.

However, for ease of programming we have restricted all step changes to halving and doubling. Thus, based on the procedure developed in [11–14], the step control procedure, which we have actually used is

$$\begin{aligned}
&\text{If } E_{\mathrm{pl}} < TOL, && h_{n+1} = 2h_n;\\
&\text{If } 100 \cdot TOL > E_{\mathrm{pl}} \geqslant TOL, && h_{n+1} = h_n;\\
&\text{If } E_{\mathrm{pl}} \geqslant 100 \cdot TOL, && h_{n+1} = \frac{h_n}{2} \text{ and repeat the step.}
\end{aligned} \tag{17}$$

We note here, that the local phase-lag error estimate is in the lower order solution y^L_{n+1}. However, if this error estimate is acceptable, i.e., less than *TOL*, we adopt the widely used procedure of performing local extrapolation. Thus, although we are actually controlling an estimate of the local error in lower phase-lag order solution y^L_{n+1}, it is the higher order solution y^H_{n+1}, which we actually accept at each point.

Now our trick to estimate the local phase-lag error in y^L_{n+1} using the phase-lag of y^H_{n+1} is clear. At every step we start with $b = 0$ and go on increasing b and checking the local phase-lag error (E_{pl}), until E_{pl} becomes less than the bound *acc* $(0 \leqslant b \leqslant \mathit{bound})$. If there is a b, for which $E_{\mathrm{pl}} < TOL$, then the step size is doubled, otherwise we carry out the integration. Moreover, when we applied our methods to our computer (i586

PC), we observed, that, if the value of *bound* was greater than 7, then (because of the round off errors) the phase-lag became of higher order than the precision of the computer used.

6.2. Coupled differential equations of the Schrödinger type

Many problems in theoretical physics and chemistry, molecular physics, atomic physics, physical chemistry, quantum chemistry, chemical physics, electronics and molecular biology can be transformed to the solution of coupled differential equations of the Schrödinger type.

The close-coupling differential equations of the Schrödinger type may be written in the form

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii}\right] y_{ij} = \sum_{m=1}^{N} V_{im} y_{mj}, \tag{18}$$

for $1 \leqslant i \leqslant N$ and $m \neq i$.

We have investigated the case, in which all channels are open. So we have the following boundary conditions (see for details [23]):

$$y_{ij} = 0 \quad \text{at } x = 0, \tag{19}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x), \tag{20}$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, respectively. We can use the present methods to problems involving close channels.

Based on the detailed analysis developed in [23] and defining a matrix K' and diagonal matrices M, N by

$$K'_{ij} = \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij}, \qquad M_{ij} = k_i x j_{l_i}(k_i x)\delta_{ij}, \qquad N_{ij} = k_i x n_{l_i}(k_i x)\delta_{ij},$$

we find that the asymptotic condition (20) may be written as

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N}\mathbf{K}'. \tag{21}$$

One of the most popular methods for the approximate solution of the coupled differential equations arising from the Schrödinger equation is the Iterative Numerov method of Allison [23].

A real problem in theoretical physics and chemistry, atomic physics, quantum chemistry and molecular physics, which can be transformed to close-coupling differential equations of the Schrödinger type is the rotational excitation of a diatomic molecule by neutral particle impact. Denoting, as in [23], the entrance channel by the quantum numbers (j, l), the exit channels by (j', l'), and the total angular momentum by $J = j + l = j' + l'$, we find that

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_{j'j}^2 - \frac{l'(l'+1)}{x^2}\right] y_{j'l'}^{Jjl}(x) = \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} \langle j'l'; J \,|\, V \,|\, j''l''; J \rangle y_{j''l''}^{Jjl}(x), \tag{22}$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2}\left[E + \frac{\hbar^2}{2I}\{j(j+1) - j'(j'+1)\}\right], \tag{23}$$

E is the kinetic energy of the incident particle in the center-of-mass system, I is the moment of inertia of the rotator, and μ is the reduced mass of the system.

Following the analysis of [23], the potential V may be written as

$$V(x, \widehat{\mathbf{k}}_{j'j}\widehat{\mathbf{k}}_{jj}) = V_0(x) P_0(\widehat{\mathbf{k}}_{j'j}\widehat{\mathbf{k}}_{jj}) + V_2(x) P_2(\widehat{\mathbf{k}}_{j'j}\widehat{\mathbf{k}}_{jj}), \tag{24}$$

and the coupling matrix element is given by

$$\langle j'l'; J \,|\, V \,|\, j''l''; J \rangle = \delta_{j'j''}\delta_{l'l''} V_0(x) + f_2(j'l', j''l''; J) V_2(x), \tag{25}$$

where the f_2 coefficients can be obtained from formulas given by Berstein et al. [24] and $\widehat{\mathbf{k}}_{j'j}$ is a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$ and P_i, $i = 0, 2$, are Legendre polynomials (see for details [24]). The boundary conditions may then be written as (see [23])

$$y_{j'l'}^{Jjl}(x) = 0 \quad \text{at } x = 0, \tag{26}$$

$$y_{j'l'}^{Jjl}(x) \sim \delta_{jj'}\delta_{ll'} \exp[-\mathrm{i}(k_{jj}x - 1/2l\pi)] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l') \exp[\mathrm{i}(k_{j'j}x - 1/2l'\pi)], \tag{27}$$

where the scattering S matrix is related to the K matrix of (20) by the relation

$$\mathbf{S} = (\mathbf{I} + \mathrm{i}\mathbf{K})(\mathbf{I} - \mathrm{i}\mathbf{K})^{-1}. \tag{28}$$

The calculation of the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles requires the existance of the numerical method for the integration from the initial value to matching points.

In our numerical test we choose the **S** matrix, which is calculated using the following parameters

$$\frac{2\mu}{\hbar^2} = 1000.0, \qquad \frac{\mu}{I} = 2.351, \qquad E = 1.1,$$
$$V_0(x) = \frac{1}{x^{12}} - 2\frac{1}{x^6}, \qquad V_2(x) = 0.2283 V_0(x).$$

As is described in [23], we take $J = 6$ and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$ and 6 giving sets of *four, nine and sixteen*

Table 3
RTC (real time of computation in seconds) in the calculation of $|S|^2$ for the variable-step methods (1)–(8). $TOL = 10^{-6}$ and *hmax* is the maximum stepsize.

Method	N	*hmax*	RTC
Iterative Numerov [23]	4	0.014	3.25
	9	0.014	23.51
	16	0.014	99.15
Variable-step method of Raptis and Cash [26]	4	0.056	1.65
	9	0.056	8.68
	16	0.056	45.21
Variable-step method of Simos [28]	4	0.448	0.29
	9	0.448	2.87
	16	0.448	11.17
RKN1 [22]	4	0.224	1.02
	9	0.224	6.33
	16	0.112	22.14
RKN2 [21]	4	0.224	0.82
	9	0.224	5.01
	16	0.224	13.43
Generator of methods of order 8 [29]	4	0.896	0.10
	9	0.896	1.04
	16	0.896	7.96
New generator of methods of order 10	4	0.896	0.06
	9	0.896	0.75
	16	0.896	6.13
Optimized generator	4	1.792	0.04
	9	0.896	0.63
	16	0.896	5.32

coupled differential equations, respectively. Following Berstein [25] and Allison [23] the reduction of the interval $[0, \infty)$ to $[0, x_0]$ is obtained. The wavefunctions are then vanished in this region and consequently the boundary condition (26) may be written as

$$y_{j'l'}^{Jjl}(x_0) = 0. \tag{29}$$

For the numerical solution of this problem we have used (1) the well-known Iterative Numerov method of Allison [23], (2) the variable-step method of Raptis and Cash [26], (3) the variable-step method developed by Simos [28], (4) the Runge–Kutta–Nyström method developed by Dormand and Prince (RKN1) (see table 13.4 of [22]), (5) the Runge–Kutta–Nyström method developed by Dormand et al. (RKN2) (see [21]), (6) the generator embedded methods of order eight [29], (7) the new generator of methods of order ten and (8) the new optimized generator. In table 3 we present the real time of computation required by the methods mentioned above to calculate the square of the modulus of the **S** matrix for sets of 4, 9 and 16 coupled differential equations. In table 3 N indicates the number of equations of the set of coupled differential equations.

In all cases the variable step procedure developed in this paper is considerably more efficient than other well known finite difference ones for a given value of hmax, so that the new family of methods can use a larger value of hmax and still gets converged results.

All computations were carried out using double precision arithmetic (16 significant digits accuracy).

Appendix. Proof of $B(s)$

For $b = 0$ $B(s)$ becomes:

$$B_0(s) = T(s) + \Big(\frac{17081263}{2^{14}3^{11}5^2}s^{12} + \frac{73363119059}{2^{17}3^{14}5^4 7}s^{14} + \frac{16305968459}{2^{18}3^{15}5^4 7}s^{16} + \frac{4596390901}{2^{21}3^{16}5^5}s^{18} + \frac{93281051}{2^{22}3^{15}5^5 7}s^{20}\Big)w_0, \tag{A.1}$$

where $T(s)$ represents:

$$T(s) = \sum_{i=0}^{5}(-1)^i \frac{1}{(2i)!}s^{2i} - \frac{112943657}{152374763520000}s^{12} - \frac{122489653693}{1645647446016000000}s^{14} - \frac{30495677389}{19747769352192000000}s^{16} - \frac{93281051}{13165179568128000000}s^{18}. \tag{A.2}$$

It is obvious that equation (A.1) is true.

For $b = v$ the formula (9) becomes:

$$B_v(s) = T(s) + \Big(\frac{17081263}{2^{20}3^{11}5^2} + \frac{73363119059}{2^{23}3^{14}5^4 7}s^2 + \frac{16305968459}{2^{24}3^{15}5^4 7}s^4 + \frac{4596390901}{2^{27}3^{16}5^5}s^6 + \frac{93281051}{2^{28}3^{15}5^5 7}s^8\Big)\sum_{i=6}^{v+6}\left[(-1)^{i+1}s^{2i}2^i\prod_{j=v}^{v+6-i}w_j\right]. \tag{A.3}$$

Assuming equation (A.3) is true, we will prove that the formula (9) for $b = v + 1$ is true. if we would set $b = v + 1$, equation (9) would become:

$$B_{v+1}(s) = T(s) + \Big(\frac{17081263}{2^{20}3^{11}5^2} + \frac{73363119059}{2^{23}3^{14}5^4 7}s^2 + \frac{16305968459}{2^{24}3^{15}5^4 7}s^4 + \frac{4596390901}{2^{27}3^{16}5^5}s^6 + \frac{93281051}{2^{28}3^{15}5^5 7}s^8\Big)\sum_{i=6}^{v+7}\left[(-1)^{i+1}s^{2i}2^i\prod_{j=v+1}^{v+7-i}w_j\right]. \tag{A.4}$$

Adding to equation (A.3) the quantity $\Theta(s)$:

$$\begin{aligned}\Theta(s) = {}&\Big(\frac{17081263}{2^{20}3^{11}5^2} + \frac{73363119059}{2^{23}3^{14}5^4 7}s^2 + \frac{16305968459}{2^{24}3^{15}5^4 7}s^4 + \frac{4596390901}{2^{27}3^{16}5^5}s^6 + \frac{93281051}{2^{28}3^{15}5^5 7}s^8\Big)\\ &\times\big[-2^6 s^{12}(w_{v+1} - w_v) + 2^7 s^{14}(w_{v+1} - w_{v-1})w_v + \cdots\\ &+ (-1)^{v+7}2^{v+6}s^{2(v+6)}(w_{v+1} - w_0)w_v w_{v-1}\cdots w_1\\ &+ (-1)^{v+8}2^{v+7}s^{2(v+7)}w_{v+1}w_v\cdots w_0\big],\end{aligned} \tag{A.5}$$

we obtain:

$$
\begin{aligned}
B_v(s) + \Theta(s) &= T(s) + \left(\tfrac{17081263}{2^{20}3^{11}5^2} + \tfrac{73363119059}{2^{23}3^{14}5^4 7}s^2 + \tfrac{16305968459}{2^{24}3^{15}5^4 7}s^4\right.\\
&\quad \left. + \tfrac{4596390901}{2^{27}3^{16}5^5}s^6 + \tfrac{93281051}{2^{28}3^{15}5^5 7}s^8\right)\\
&\quad \times \left(\sum_{i=6}^{v+6}\left[(-1)^{i+1}s^{2i}2^i\prod_{j=v}^{v+6-i} w_j\right] - 2^6 s^{12}(w_{v+1} - w_v)\right.\\
&\quad \left. + 2^7 s^{14}(w_{v+1} - w_{v-1})w_v + \cdots + (-1)^{v+8}2^{v+7}s^{2(v+7)}w_{v+1}w_v\cdots w_0\right)\\
&= T(s) + \left(\tfrac{17081263}{2^{20}3^{11}5^2} + \tfrac{73363119059}{2^{23}3^{14}5^4 7}s^2\right.\\
&\quad \left. + \tfrac{16305968459}{2^{24}3^{15}5^4 7}s^4 + \tfrac{4596390901}{2^{27}3^{16}5^5}s^6 + \tfrac{93281051}{2^{28}3^{15}5^5 7}s^8\right)\\
&\quad \times \left[-2^6 s^{12}w_v + 2^7 s^{14}w_{v-1}w_v + \cdots\right.\\
&\quad + (-1)^{v+7}2^{v+6}s^{2(v+6)}w_v w_{v-1}\cdots w_0\\
&\quad - 2^6 s^{12}(w_{v+1} - w_v) + 2^7 s^{14}(w_{v+1} - w_{v-1})w_v + \cdots\\
&\quad + (-1)^{v+7}2^{v+6}s^{2(v+6)}(w_{v+1} - w_0)w_v w_{v-1}\cdots w_1\\
&\quad \left. + (-1)^{v+8}2^{v+7}s^{2(v+7)}w_{v+1}w_v\cdots w_0\right]\\
&= \sum_{i=0}^{5}(-1)^i\tfrac{1}{(2i)!}s^{2i} - \tfrac{112943657}{152374763520000}s^{12} - \tfrac{122489653693}{1645647446016000000}s^{14}\\
&\quad - \tfrac{30495677389}{19747769352192000000}s^{16} - \tfrac{93281051}{13165179568128000000}s^{18}\\
&\quad + \left(\tfrac{17081263}{2^{20}3^{11}5^2} + \tfrac{73363119059}{2^{23}3^{14}5^4 7}s^2 + \tfrac{16305968459}{2^{24}3^{15}5^4 7}s^4 + \tfrac{4596390901}{2^{27}3^{16}5^5}s^6 + \tfrac{93281051}{2^{28}3^{15}5^5 7}s^8\right)\\
&\quad \times \left(-2^6 s^{12}w_{v+1} + \cdots + (-1)^{v+8}2^{v+7}s^{2(v+7)}w_{v+1}\cdots w_0\right). \qquad \text{(A.6)}
\end{aligned}
$$

Based on the previous, we can see that equation (A.6) is equivalent to equation (A.4). So, if we add $\Theta(s)$ to $B(s)$ (for any $b = v$), we obtain the next $B(s)$ (for $b = v + 1$). Thus the formula has been proved.

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