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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 1. Development of the basic method *

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In this paper we present the development of a generator of hybrid explicit methods for the numerical solution of the Schrödinger equation. The methods are of algebraic order ten. The coefficients of the generator are calculated appropriately.

KEY WORDS: hybrid methods, explicit methods, algebraic order, periodic problems, initial-value problems, Schrödinger equation

1. Introduction

During the last two decades, great interest has been observed [1–16], for the numerical solution of special second order periodic initial-value problems of the form:

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

Scattering or eigenvalue problems and generally problems with oscillating solutions, which can be expressed in the form of equation (1) or in systems of equations of the form (1), can be found in scientific areas, such as theoretical physics, quantum mechanics, atomic physics, molecular physics, theoretical chemistry, astrophysics, chemical physics, electronics and elsewhere (see [17,18]).

The maximum algebraic order, the maximum phase-lag order and the maximum interval of periodicity are the main characteristics of the numerical methods, used in the solution of the above problems. The development of methods with the above properties

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is a problem of great interest for many researchers. Numerov's method is the most popular method for the numerical solution of the above problems.

The last few years a great research activity is observed in the construction of methods with minimal phase-lag. We refer to the methods of Simos et al. [1,9,10,13,14,19, 20], Chawla et al. [4–7], Coleman [8] and Avdelas et al. [11,12]. In [9] Simos and Raptis have combined the properties of phase-lag and P-stability (a method is called P-stable, when its interval of periodicity is equal to $(0, \infty)$). Simos [20] and Avdelas et al. [21] have developed families of eighth algebraic order explicit methods for the solution of problems of the form (1).

The radial Schrödinger equation has been a subject of great importance in numerous scientific fields. There is a real need for its numerical solution in nuclear physics, physical chemistry, theoretical physics and chemistry, quantum chemistry and molecular physics. During the last decade, great activity is observed in developing numerical methods for the radial Schrödinger equation (see [22–28]). This equation has the following form:

$$y''(x) + f(x)y(x) = 0, \tag{2}$$

where x is the radius with $0 \leqslant x < \infty$ and $f(x) = E - l(l+1)/x^2 - V(x)$. We call the term $l(l+1)/x^2$ *the centrifugal potential*, and the function $V(x)$ *the potential*, where $V(x) \to 0$ as $x \to \infty$. According to the sign of the energy E, there are two main categories of problems for equation (2) (see for details [16]). In equation (2) E is a real number denoting *the energy*, l is a given integer and V is a given function, which denotes *the potential*. The function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$. The first boundary condition is

$$y(0) = 0 \tag{3}$$

and a second boundary condition for large values of x, is determined by physical considerations.

In this paper the development of a generator of tenth algebraic order explicit methods is presented. 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. In sections 2 and 3 the construction of the main part of the generator of methods and the local truncation error are given.

2. Development of the new method

We consider the following family of methods.

$$\begin{aligned}
\overline{y}_{n+k} &= (r_{00}y_{n+1} + r_{01}y_n + r_{02}y_{n-1}) + h^2(r_{03}f_{n+1} + r_{04}f_n + r_{05}f_{n-1}),\\
\overline{f}_{n+k} &= f(x_{n+k}, \overline{y}_{n+k}), \quad k = \tfrac{1}{2},\\
\overline{y}_{n-k} &= (r_{10}y_{n+1} + r_{11}y_n + r_{12}y_{n-1}) + h^2(r_{13}f_{n+1} + r_{14}f_n + r_{15}f_{n-1}),
\end{aligned} \tag{4}$$

$$\overline{f}_{n-k} = f\left(x_{n-k}, \overline{y}_{n-k}\right), \quad k = \tfrac{1}{2}, \tag{5}$$

$$\begin{aligned} \overline{y}_{n+l} &= (k_{00} y_{n+1} + k_{01} y_n + k_{02} y_{n-1}) \\ &\quad + h^2 (k_{03} f_{n+1} + k_{04} f_n + k_{05} f_{n-1} + k_{06} f_{n+k} + k_{07} f_{n-k}), \end{aligned}$$

$$\overline{f}_{n+l} = f\left(x_{n+l}, \overline{y}_{n+l}\right), \quad l = \tfrac{1}{4}, \tag{6}$$

$$\begin{aligned} \overline{y}_{n-l} &= (k_{10} y_{n+1} + k_{11} y_n + k_{12} y_{n-1}) \\ &\quad + h^2 (k_{13} f_{n+1} + k_{14} f_n + k_{15} f_{n-1} + k_{16} f_{n+k} + k_{17} f_{n-k}), \end{aligned}$$

$$\overline{f}_{n-l} = f\left(x_{n-l}, \overline{y}_{n-l}\right), \quad l = \tfrac{1}{4}, \tag{7}$$

$$\overline{y}_{n_i} = y_n - w_i h^2 (f_{n+1} - 2 f_n + f_{n-1}), \quad i = 0(1)b, \tag{8}$$

$$\begin{aligned} \overline{y}_{n+1} &= 2 y_n - y_{n-1} \\ &\quad + h^2 \left[t_0 (f_{n+1} + f_{n-1}) + t_1 \overline{f}_n + t_2 \left(\overline{f}_{n+1/2} + \overline{f}_{n-1/2} \right) + t_3 \left(\overline{f}_{n+1/4} + \overline{f}_{n-1/4} \right) \right], \end{aligned} \tag{9}$$

where b denotes each method of the family and is defined by the user.

In order to define the coefficients of the above family of methods we act as follows.

(i) We define the following approximations:

$$y_{n+k} + y_{n-k} = m_0 (y_{n+1} + y_{n-1}) + m_1 y_n + h^2 \left[m_2 (f_{n+1} + f_{n-1}) + m_3 f_n \right], \tag{10}$$

$$y_{n+k} - y_{n-k} = n_0 (y_{n+1} - y_{n-1}) + h^2 n_1 (f_{n+1} - f_{n-1}), \tag{11}$$

$$\begin{aligned} y_{n+l} + y_{n-l} &= p_0 (y_{n+1} + y_{n-1}) + p_1 y_n \\ &\quad + h^2 \left[p_2 (f_{n+1} + f_{n-1}) + p_3 f_n + p_4 (f_{n+k} + f_{n-k}) \right], \end{aligned} \tag{12}$$

$$y_{n+l} - y_{n-l} = q_0 (y_{n+1} - y_{n-1}) + h^2 \left[q_1 (f_{n+1} - f_{n-1}) + q_2 (f_{n+k} - f_{n-k}) \right]. \tag{13}$$

(ii) For $k = 1/2$ and $l = 1/4$, we expand $y_{n\pm 1}$, $y_{n\pm k}$, $y_{n\pm l}$, $f_{n\pm 1}$, $f_{n\pm k}$ and $f_{n\pm l}$ via Taylor series and we define the coefficients of the formulae (10)–(13), in order to have reduced local truncation errors, from a set of systems of equations, which are the following.

For equation (10) we obtain

$$2 - 2m_0 - m_1 = 0, \tag{14}$$

$$\tfrac{1}{4} - m_0 - 2m_2 - m_3 = 0, \tag{15}$$

$$\tfrac{1}{192} - \tfrac{1}{12} m_0 - m_2 = 0, \tag{16}$$

$$\tfrac{1}{23040} - \tfrac{1}{360} m_0 - \tfrac{1}{12} m_2 = 0. \tag{17}$$

For equation (11) we obtain

$$1 - 2n_0 = 0, \tag{18}$$

$$\tfrac{1}{24} - \tfrac{1}{3} n_0 - 2n_1 = 0. \tag{19}$$

For equation (12) we obtain

$$2-2p_0-p_1=0, \tag{20}$$
$$\tfrac{1}{16}-p_0-2p_2-p_3-2p_4=0, \tag{21}$$
$$\tfrac{1}{3072}-\tfrac{1}{12}p_0-p_2-\tfrac{1}{4}p_4=0, \tag{22}$$
$$\tfrac{1}{1474560}-\tfrac{1}{360}p_0-\tfrac{1}{12}p_2-\tfrac{1}{192}p_4=0, \tag{23}$$
$$\tfrac{1}{1321205760}-\tfrac{1}{20160}p_0-\tfrac{1}{360}p_2-\tfrac{1}{23040}p_4=0. \tag{24}$$

For equation (13) we obtain

$$\tfrac{1}{2}-2q_0=0, \tag{25}$$
$$\tfrac{1}{192}-\tfrac{1}{3}q_0-2q_1-q_2=0, \tag{26}$$
$$\tfrac{1}{61440}-\tfrac{1}{60}q_0-\tfrac{1}{3}q_1-\tfrac{1}{24}q_2=0. \tag{27}$$

Solving the above systems of equations, we obtain the coefficients of the formulae (10)–(13), presented below:

$$m_0=\tfrac{3}{32},\quad m_1=\tfrac{29}{16},\quad m_2=-\tfrac{1}{384},\quad m_3=\tfrac{31}{192},$$
$$n_0=\tfrac{1}{2},\quad n_1=-\tfrac{1}{16},$$
$$p_0=-\tfrac{787}{32768},\quad p_1=\tfrac{33555}{16384},\quad p_2=\tfrac{119}{393216},\quad p_3=\tfrac{4569}{65536},\quad p_4=\tfrac{199}{24576},$$
$$q_0=\tfrac{1}{4},\quad q_1=-\tfrac{11}{3072},\quad q_2=-\tfrac{109}{1536}.$$

(iii) By addition and subtraction of equations (10)–(13), the parameters of equations (4)–(7) are obtained.

(iv) We substitute $y_{n\pm1}, y_{n\pm1/2}, y_{n\pm1/4}$ and $f_{n\pm1}, f_{n\pm1/2}, f_{n\pm1/4}$ in (9) with their Taylor series expansions and we obtain the following system of equations:

$$1-2t_0-t_1-2t_2-2t_3=0, \tag{28}$$
$$\tfrac{1}{12}-t_0-\tfrac{1}{4}t_2-\tfrac{1}{16}t_3=0, \tag{29}$$
$$\tfrac{1}{360}-\tfrac{1}{12}t_0-\tfrac{1}{192}t_2-\tfrac{1}{3072}t_3=0, \tag{30}$$
$$\tfrac{1}{20160}-\tfrac{1}{360}t_0-\tfrac{1}{23040}t_2-\tfrac{1}{1474560}t_3=0. \tag{31}$$

(v) We add to the family, given at the beginning of this section, the layers given below:

$$\begin{aligned}\tilde{y}_{n+1/2}={}&a_{00}\overline{y}_{n+1}+a_{01}y_n+a_{02}y_{n-1}+h^2\big(a_{03}\overline{f}_{n+1}+a_{04}f_n\\&+a_{05}f_{n-1}+a_{06}\overline{f}_{n+1/2}+a_{07}\overline{f}_{n-1/2}+a_{08}\overline{f}_{n+1/4}+a_{09}\overline{f}_{n-1/4}\big),\end{aligned} \tag{32}$$
$$\begin{aligned}\tilde{y}_{n-1/2}={}&a_{10}\overline{y}_{n+1}+a_{11}y_n+a_{12}y_{n-1}+h^2\big(a_{13}\overline{f}_{n+1}+a_{14}f_n\\&+a_{15}f_{n-1}+a_{16}\overline{f}_{n+1/2}+a_{17}\overline{f}_{n-1/2}+a_{18}\overline{f}_{n+1/4}+a_{19}\overline{f}_{n-1/4}\big),\end{aligned} \tag{33}$$
$$\begin{aligned}\tilde{y}_{n+1/4}={}&c_{00}\overline{y}_{n+1}+c_{01}y_n+c_{02}y_{n-1}+h^2\big(c_{03}\overline{f}_{n+1}+c_{04}f_n\\&+c_{05}f_{n-1}+c_{06}\overline{f}_{n+1/2}+c_{07}\overline{f}_{n-1/2}+c_{08}\overline{f}_{n+1/4}+c_{09}\overline{f}_{n-1/4}\big),\end{aligned} \tag{34}$$

$$\widetilde{y}_{n-1/4} = c_{10}\overline{y}_{n+1} + c_{11}y_n + c_{12}y_{n-1} + h^2\big(c_{13}\overline{f}_{n+1} + c_{14}f_n + c_{15}f_{n-1} + c_{16}\overline{f}_{n+1/2} + c_{17}\overline{f}_{n-1/2} + c_{18}\overline{f}_{n+1/4} + c_{19}\overline{f}_{n-1/4}\big), \tag{35}$$

$$\widetilde{y}_{n+1/8} = e_{00}\overline{y}_{n+1} + e_{01}y_n + e_{02}y_{n-1} + h^2\big(e_{03}\overline{f}_{n+1} + e_{04}f_n + e_{05}f_{n-1} + e_{06}\overline{f}_{n+1/2} + e_{07}\overline{f}_{n-1/2} + e_{08}\overline{f}_{n+1/4} + e_{09}\overline{f}_{n-1/4}\big), \tag{36}$$

$$\widetilde{y}_{n-1/8} = e_{10}\overline{y}_{n+1} + e_{11}y_n + e_{12}y_{n-1} + h^2\big(e_{13}\overline{f}_{n+1} + e_{14}f_n + e_{15}f_{n-1} + e_{16}\overline{f}_{n+1/2} + e_{17}\overline{f}_{n-1/2} + e_{18}\overline{f}_{n+1/4} + e_{19}\overline{f}_{n-1/4}\big), \tag{37}$$

$$y_{n+1} - 2y_n + y_{n-1} = h^2\big[g_0\big(\overline{f}_{n+1} + f_{n-1}\big) + g_1 f_n + g_2\big(\widetilde{f}_{n+1/2} + \widetilde{f}_{n-1/2}\big) + g_3\big(\widetilde{f}_{n+1/4} + \widetilde{f}_{n-1/4}\big) + g_4\big(\widetilde{f}_{n+1/8} + \widetilde{f}_{n-1/8}\big)\big]. \tag{38}$$

(vi) We work in the same way as above. The quantities $y_{n\pm1}$, $y_{n\pm1/2}$, $y_{n\pm1/4}$, $y_{n\pm1/8}$ and f_{n+1}, $f_{n\pm1/2}$, $f_{n\pm1/4}$, $f_{n\pm1/8}$ are replaced by their Taylor series expansions in equations (32)–(38). From the coefficients of the first powers of h, a system of equations, corresponding to each layer, arises. Solving these systems of equations, the unknown parameters are obtained.

System extracted from equation (32):

$$1 - a_{02} - a_{00} - a_{01} = 0, \tag{39}$$

$$\tfrac{1}{2} - a_{00} + a_{02} = 0, \tag{40}$$

$$\tfrac{1}{8} - a_{06} - a_{09} - a_{05} - a_{07} - a_{03} - \tfrac{1}{2}a_{00} - \tfrac{1}{2}a_{02} - a_{08} - a_{04} = 0, \tag{41}$$

$$\tfrac{1}{48} - \tfrac{1}{2}a_{06} - \tfrac{1}{6}a_{00} + \tfrac{1}{6}a_{02} - a_{03} + a_{05} + \tfrac{1}{2}a_{07} - \tfrac{1}{4}a_{08} + \tfrac{1}{4}a_{09} = 0, \tag{42}$$

$$\tfrac{1}{384} - \tfrac{1}{24}a_{00} - \tfrac{1}{8}a_{07} - \tfrac{1}{2}a_{03} - \tfrac{1}{2}a_{05} - \tfrac{1}{8}a_{06} - \tfrac{1}{32}a_{08} - \tfrac{1}{32}a_{09} - \tfrac{1}{24}a_{02} = 0, \tag{43}$$

$$\tfrac{1}{3840} - \tfrac{1}{120}a_{00} - \tfrac{1}{6}a_{03} - \tfrac{1}{48}a_{06} + \tfrac{1}{48}a_{07} - \tfrac{1}{384}a_{08} + \tfrac{1}{384}a_{09} + \tfrac{1}{120}a_{02} + \tfrac{1}{6}a_{05} = 0, \tag{44}$$

$$\tfrac{1}{46080} - \tfrac{1}{720}a_{00} - \tfrac{1}{24}a_{03} - \tfrac{1}{384}a_{06} - \tfrac{1}{384}a_{07} - \tfrac{1}{6144}a_{08} - \tfrac{1}{6144}a_{09} - \tfrac{1}{720}a_{02} - \tfrac{1}{24}a_{05} = 0, \tag{45}$$

$$\tfrac{1}{645120} - \tfrac{1}{5040}a_{00} - \tfrac{1}{120}a_{03} - \tfrac{1}{3840}a_{06} + \tfrac{1}{3840}a_{07} - \tfrac{1}{122880}a_{08} + \tfrac{1}{122880}a_{09} + \tfrac{1}{5040}a_{02} + \tfrac{1}{10}a_{05} = 0, \tag{46}$$

$$\tfrac{1}{10321920} - \tfrac{1}{40320}a_{00} - \tfrac{1}{720}a_{03} - \tfrac{1}{46080}a_{06} - \tfrac{1}{46080}a_{07} - \tfrac{1}{2949120}a_{08} - \tfrac{1}{2949120}a_{09} - \tfrac{1}{40320}a_{02} - \tfrac{1}{720}a_{05} = 0, \tag{47}$$

$$\tfrac{1}{185794560} + \tfrac{1}{362880}a_{02} - \tfrac{1}{362880}a_{00} - \tfrac{1}{5040}a_{03} - \tfrac{1}{645120}a_{06} + \tfrac{1}{645120}a_{07} - \tfrac{1}{82575360}a_{08} + \tfrac{1}{82575360}a_{09} + \tfrac{1}{5040}a_{05} = 0. \tag{48}$$

System extracted from equation (33):

$$1 - a_{10} - a_{12} - a_{11} = 0, \tag{49}$$

$$-a_{10} + a_{12} - \tfrac{1}{2} = 0, \tag{50}$$

$$-a_{14} - a_{15} - a_{13} - \tfrac{1}{2}a_{12} - a_{19} - a_{18} - a_{17} - a_{16} - \tfrac{1}{2}a_{10} + \tfrac{1}{8} = 0, \tag{51}$$

$$a_{15} - a_{13} - \tfrac{1}{4}a_{18} + \tfrac{1}{6}a_{12} + \tfrac{1}{4}a_{19} - \tfrac{1}{2}a_{16} + \tfrac{1}{2}a_{17} - \tfrac{1}{6}a_{10} - \tfrac{1}{48} = 0, \tag{52}$$

$$-\tfrac{1}{2}a_{15} - \tfrac{1}{2}a_{13} - \tfrac{1}{24}a_{12} - \tfrac{1}{32}a_{19} - \tfrac{1}{8}a_{16} - \tfrac{1}{32}a_{18} - \tfrac{1}{8}a_{17} - \tfrac{1}{24}a_{10} + \tfrac{1}{384} = 0, \tag{53}$$

$$\tfrac{1}{6}a_{15} - \tfrac{1}{6}a_{13} + \tfrac{1}{120}a_{12} + \tfrac{1}{384}a_{19} - \tfrac{1}{384}a_{18} - \tfrac{1}{48}a_{16} + \tfrac{1}{48}a_{17} - \tfrac{1}{120}a_{10} - \tfrac{1}{3840} = 0, \tag{54}$$

$$-\tfrac{1}{6144}a_{18} - \tfrac{1}{24}a_{13} - \tfrac{1}{720}a_{12} - \tfrac{1}{6144}a_{19} - \tfrac{1}{384}a_{16} - \tfrac{1}{384}a_{17} - \tfrac{1}{720}a_{10} - \tfrac{1}{24}a_{15} + \tfrac{1}{46080} = 0, \tag{55}$$

$$-\tfrac{1}{122880}a_{18} - \tfrac{1}{120}a_{13} + \tfrac{1}{5040}a_{12} + \tfrac{1}{122880}a_{19} + \tfrac{1}{3840}a_{17} + \tfrac{1}{120}a_{15} - \tfrac{1}{3840}a_{16} - \tfrac{1}{5040}a_{10} - \tfrac{1}{645120} = 0, \tag{56}$$

$$-\tfrac{1}{2949120}a_{18} - \tfrac{1}{720}a_{13} - \tfrac{1}{40320}a_{12} - \tfrac{1}{2949120}a_{19} - \tfrac{1}{46080}a_{17} - \tfrac{1}{46080}a_{16} - \tfrac{1}{40320}a_{10} - \tfrac{1}{720}a_{15} + \tfrac{1}{10321920} = 0, \tag{57}$$

$$-\tfrac{1}{82575360}a_{18} - \tfrac{1}{5040}a_{13} + \tfrac{1}{362880}a_{12} + \tfrac{1}{82575360}a_{19} + \tfrac{1}{645120}a_{17} + \tfrac{1}{5040}a_{15} - \tfrac{1}{645120}a_{16} - \tfrac{1}{362880}a_{10} - \tfrac{1}{185794560} = 0. \tag{58}$$

System extracted from equation (34):

$$1 - c_{02} - c_{00} - c_{01} = 0, \tag{59}$$

$$\tfrac{1}{4} - c_{00} + c_{02} = 0, \tag{60}$$

$$\tfrac{1}{32} - c_{09} - c_{04} - c_{08} - c_{07} - c_{06} - c_{05} - c_{03} - \tfrac{1}{2}c_{00} - \tfrac{1}{2}c_{02} = 0, \tag{61}$$

$$\tfrac{1}{384} + \tfrac{1}{4}c_{09} - c_{03} + c_{05} - \tfrac{1}{6}c_{00} + \tfrac{1}{6}c_{02} - \tfrac{1}{2}c_{06} + \tfrac{1}{2}c_{07} - \tfrac{1}{4}c_{08} = 0, \tag{62}$$

$$\tfrac{1}{6144} - \tfrac{1}{32}c_{09} - \tfrac{1}{2}c_{03} - \tfrac{1}{2}c_{05} - \tfrac{1}{24}c_{00} - \tfrac{1}{24}c_{02} - \tfrac{1}{8}c_{06} - \tfrac{1}{r8}c_{07} - \tfrac{1}{32}c_{08} = 0, \tag{63}$$

$$\tfrac{1}{122880} + \tfrac{1}{384}c_{09} - \tfrac{1}{6}c_{03} + \tfrac{1}{6}c_{05} + \tfrac{1}{120}c_{02} - \tfrac{1}{120}c_{00} - \tfrac{1}{48}c_{06} + \tfrac{1}{48}c_{07} - \tfrac{1}{384}c_{08} = 0, \tag{64}$$

$$\tfrac{1}{2949120} - \tfrac{1}{6144}c_{09} - \tfrac{1}{24}c_{03} - \tfrac{1}{24}c_{05} - \tfrac{1}{720}c_{02} - \tfrac{1}{384}c_{07} - \tfrac{1}{720}c_{00} - \tfrac{1}{384}c_{06} - \tfrac{1}{6144}c_{08} = 0, \tag{65}$$

$$\tfrac{1}{82575360} + \tfrac{1}{122880}c_{09} - \tfrac{1}{120}c_{03} + \tfrac{1}{5040}c_{02} - \tfrac{1}{5040}c_{00} - \tfrac{1}{3840}c_{06} + \tfrac{1}{120}c_{05} + \tfrac{1}{3840}c_{07} - \tfrac{1}{122880}c_{08} = 0, \tag{66}$$

$$\tfrac{1}{2642411520} - \tfrac{1}{2949120}c_{09} - \tfrac{1}{720}c_{03} - \tfrac{1}{720}c_{05} - \tfrac{1}{40320}c_{02} - \tfrac{1}{40320}c_{00} - \tfrac{1}{46080}c_{06} - \tfrac{1}{46080}c_{07} - \tfrac{1}{2949120}c_{08} = 0, \tag{67}$$

$$\tfrac{1}{95126814720} - \tfrac{1}{82575360}c_{08} + \tfrac{1}{82575360}c_{09} - \tfrac{1}{5040}c_{03} + \tfrac{1}{5040}c_{05} + \tfrac{1}{362880}c_{02} - \tfrac{1}{362880}c_{00} - \tfrac{1}{645120}c_{06} + \tfrac{1}{645120}c_{07} = 0. \tag{68}$$

System extracted from equation (35):

$$1 - c_{10} - c_{12} - c_{11} = 0, \tag{69}$$

$$-\tfrac{1}{4} + c_{12} - c_{10} = 0, \tag{70}$$

$$\tfrac{1}{32} - \tfrac{1}{2}c_{12} - \tfrac{1}{2}c_{10} - c_{19} - c_{18} - c_{17} - c_{16} - c_{15} - c_{13} - c_{14} = 0, \tag{71}$$

$$-\tfrac{1}{384} - c_{13} + \tfrac{1}{4}c_{19} + \tfrac{1}{2}c_{17} + \tfrac{1}{6}c_{12} - \tfrac{1}{6}c_{10} - \tfrac{1}{4}c_{18} - \tfrac{1}{2}c_{16} + c_{15} = 0, \tag{72}$$

$$\frac{1}{6144} - \frac{1}{2}c_{13} - \frac{1}{32}c_{19} - \frac{1}{8}c_{17} - \frac{1}{24}c_{12} - \frac{1}{24}c_{10} - \frac{1}{32}c_{18} - \frac{1}{8}c_{16} - \frac{1}{2}c_{15} = 0, \quad (73)$$

$$-\frac{1}{122880} - \frac{1}{6}c_{13} + \frac{1}{384}c_{19} + \frac{1}{48}c_{17} + \frac{1}{120}c_{12} - \frac{1}{120}c_{10} - \frac{1}{384}c_{18} - \frac{1}{48}c_{16} + \frac{1}{6}c_{15} = 0, \quad (74)$$

$$\frac{1}{2949120} - \frac{1}{24}c_{13} - \frac{1}{6144}c_{19} - \frac{1}{384}c_{17} - \frac{1}{720}c_{12} - \frac{1}{720}c_{10} - \frac{1}{6144}c_{18} - \frac{1}{384}c_{16} - \frac{1}{24}c_{15} = 0, \quad (75)$$

$$-\frac{1}{82575360} - \frac{1}{120}c_{13} + \frac{1}{122880}c_{19} + \frac{1}{3840}c_{17} - \frac{1}{5040}c_{10} + \frac{1}{5040}c_{12} - \frac{1}{122880}c_{18} - \frac{1}{3840}c_{16} + \frac{1}{120}c_{15} = 0, \quad (76)$$

$$\frac{1}{2642411520} - \frac{1}{2949120}c_{19} - \frac{1}{46080}c_{17} - \frac{1}{720}c_{13} - \frac{1}{40320}c_{10} - \frac{1}{40320}c_{12} - \frac{1}{2949120}c_{18} - \frac{1}{46080}c_{16} - \frac{1}{720}c_{15} = 0, \quad (77)$$

$$-\frac{1}{95126814720} + \frac{1}{645120}c_{17} - \frac{1}{362880}c_{10} + \frac{1}{362880}c_{12} + \frac{1}{82575360}c_{19} - \frac{1}{82575360}c_{18} - \frac{1}{645120}c_{16} - \frac{1}{5040}c_{13} + \frac{1}{5040}c_{15} = 0. \quad (78)$$

System extracted from equation (36):

$$1 - e_{01} - e_{02} - e_{00} = 0, \quad (79)$$

$$\frac{1}{8} - e_{00} + e_{02} = 0, \quad (80)$$

$$\frac{1}{128} - \frac{1}{2}e_{00} - \frac{1}{2}e_{02} - e_{07} - e_{09} - e_{04} - e_{03} - e_{06} - e_{05} - e_{08} = 0, \quad (81)$$

$$\frac{1}{3072} + \frac{1}{4}e_{09} - \frac{1}{4}e_{08} + \frac{1}{2}e_{07} - e_{03} + e_{05} + \frac{1}{6}e_{02} - \frac{1}{2}e_{06} - \frac{1}{6}e_{00} = 0, \quad (82)$$

$$\frac{1}{98304} - \frac{1}{32}e_{09} - \frac{1}{32}e_{08} - \frac{1}{8}e_{07} - \frac{1}{8}e_{06} - \frac{1}{2}e_{03} - \frac{1}{2}e_{05} - \frac{1}{24}e_{02} - \frac{1}{24}e_{00} = 0, \quad (83)$$

$$\frac{1}{3932160} - \frac{1}{384}e_{08} + \frac{1}{384}e_{09} + \frac{1}{48}e_{07} - \frac{1}{48}e_{06} - \frac{1}{6}e_{03} + \frac{1}{6}e_{05} + \frac{1}{120}e_{02} - \frac{1}{120}e_{00} = 0, \quad (84)$$

$$\frac{1}{188743680} - \frac{1}{6144}e_{09} - \frac{1}{6144}e_{08} - \frac{1}{384}e_{07} - \frac{1}{384}e_{06} - \frac{1}{24}e_{03} - \frac{1}{24}e_{05} - \frac{1}{720}e_{02} - \frac{1}{720}e_{00} = 0, \quad (85)$$

$$\frac{1}{10569646080} - \frac{1}{122880}e_{08} + \frac{1}{122880}e_{09} + \frac{1}{3840}e_{07} - \frac{1}{3840}e_{06} + \frac{1}{120}e_{05} - \frac{1}{120}e_{03} + \frac{1}{5040}e_{02} - \frac{1}{5040}e_{00} = 0, \quad (86)$$

$$\frac{1}{676457349120} - \frac{1}{2949120}e_{08} - \frac{1}{46080}e_{06} - \frac{1}{720}e_{05} - \frac{1}{46080}e_{07} - \frac{1}{720}e_{03} - \frac{1}{40320}e_{02} - \frac{1}{2949120}e_{09} - \frac{1}{40320}e_{00} = 0, \quad (87)$$

$$\frac{1}{48704929136640} - \frac{1}{82575360}e_{08} + \frac{1}{645120}e_{07} - \frac{1}{645120}e_{06} + \frac{1}{5040}e_{05} - \frac{1}{5040}e_{03} - \frac{1}{362880}e_{00} + \frac{1}{362880}e_{02} + \frac{1}{82575360}e_{09} = 0. \quad (88)$$

System extracted from equation (37):

$$1 - e_{10} - e_{12} - e_{11} = 0, \quad (89)$$

$$-\frac{1}{8} + e_{12} - e_{10} = 0, \quad (90)$$

$$\frac{1}{128} - \frac{1}{2}e_{12} - \frac{1}{2}e_{10} - e_{15} - e_{16} - e_{17} - e_{13} - e_{18} - e_{19} - e_{14} = 0, \quad (91)$$

$$-\frac{1}{3072} + e_{15} + \frac{1}{6}e_{12} - \frac{1}{6}e_{10} - e_{13} - \frac{1}{4}e_{18} + \frac{1}{4}e_{19} - \frac{1}{2}e_{16} + \frac{1}{2}e_{17} = 0, \quad (92)$$

$$\frac{1}{98304}-\frac{1}{32}e_{18}-\frac{1}{2}e_{15}-\frac{1}{24}e_{12}-\frac{1}{24}e_{10}-\frac{1}{2}e_{13}-\frac{1}{32}e_{19}-\frac{1}{8}e_{16}-\frac{1}{8}e_{17}=0, \tag{93}$$

$$-\frac{1}{3932160}-\frac{1}{384}e_{18}+\frac{1}{6}e_{15}+\frac{1}{120}e_{12}-\frac{1}{120}e_{10}-\frac{1}{6}e_{13}+\frac{1}{384}e_{19} -\frac{1}{48}e_{16}+\frac{1}{48}e_{17}=0, \tag{94}$$

$$\frac{1}{188743680}-\frac{1}{6144}e_{18}-\frac{1}{24}e_{15}-\frac{1}{720}e_{12}-\frac{1}{720}e_{10}-\frac{1}{24}e_{13}-\frac{1}{6144}e_{19} -\frac{1}{384}e_{16}-\frac{1}{384}e_{17}=0, \tag{95}$$

$$-\frac{1}{10569646080}-\frac{1}{122880}e_{18}+\frac{1}{120}e_{15}+\frac{1}{5040}e_{12}-\frac{1}{5040}e_{10}-\frac{1}{120}e_{13}+\frac{1}{122880}e_{19} -\frac{1}{3840}e_{16}+\frac{1}{3840}e_{17}=0, \tag{96}$$

$$\frac{1}{676457349120}-\frac{1}{2949120}e_{18}-\frac{1}{40320}e_{12}-\frac{1}{40320}e_{10}-\frac{1}{720}e_{13}-\frac{1}{46080}e_{17}-\frac{1}{2949120}e_{19} -\frac{1}{720}e_{15}-\frac{1}{46080}e_{16}=0, \tag{97}$$

$$-\frac{1}{48704929136640}-\frac{1}{82575360}e_{18}+\frac{1}{362880}e_{12}-\frac{1}{362880}e_{10}-\frac{1}{5040}e_{13}+\frac{1}{645120}e_{17} +\frac{1}{82575360}e_{19}+\frac{1}{5040}e_{15}-\frac{1}{645120}e_{16}=0. \tag{98}$$

System extracted from equation (38):

$$1-2g_4-2g_3-2g_2-2g_0-g_1=0, \tag{99}$$

$$\frac{1}{12}-\frac{1}{16}g_3-\frac{1}{64}g_4-\frac{1}{4}g_2-g_0=0, \tag{100}$$

$$\frac{1}{360}-\frac{1}{192}g_2-\frac{1}{3072}g_3-\frac{1}{49152}g_4-\frac{1}{12}g_0=0, \tag{101}$$

$$\frac{1}{20160}-\frac{1}{23040}g_2-\frac{1}{1474560}g_3-\frac{1}{94371840}g_4-\frac{1}{360}g_0=0, \tag{102}$$

$$\frac{1}{1814400}-\frac{1}{5160960}g_2-\frac{1}{1321205760}g_3-\frac{1}{338228674560}g_4-\frac{1}{20160}g_0=0. \tag{103}$$

Attempting to solve the above systems, we observe that free parameters exist. So, in the cases of equations (32), (34) and (36) we set $a_{02}=0$, $c_{02}=0$ and $e_{02}=0$ and for equations (33), (35) and (37) we set $a_{10}=0$, $c_{10}=0$ and $e_{10}=0$.

3. The new generator of methods

Based on the previous section and solving the above systems of equations, we obtain the coefficients of the new generator of methods. So, we consider the following final form of the family of methods:

$$\overline{y}_{n+1}=2y_n-y_{n-1}+h^2f_n+\mathrm{O}\big(h^4\big), \tag{104}$$

$$\overline{y}_{n_i}=y_n-w_ih^2\big(\overline{f}_{n+1}-2f_n+f_{n-1}\big)+\mathrm{O}\big(h^4\big), \tag{105}$$

$$\widetilde{y}_{n+1}=2y_n-y_{n-1}+\frac{h^2}{12}\big(\overline{f}_{n+1}+10\overline{f}_{n_i}+f_{n-1}\big)+\mathrm{O}\big(h^6\big), \tag{106}$$

$$\overline{y}_{n+1/2}=\frac{1}{64}\big(19\widetilde{y}_{n+1}+58y_n-13y_{n-1}\big)+\frac{h^2}{768}\big(-25\widetilde{f}_{n+1}+62f_n+23f_{n-1}\big) +\mathrm{O}\big(h^6\big), \tag{107}$$

$$\overline{y}_{n-1/2}=\frac{1}{64}\big(-13\widetilde{y}_{n+1}+58y_n+19y_{n-1}\big)+\frac{h^2}{768}\big(23\widetilde{f}_{n+1}+62f_n-25f_{n-1}\big) +\mathrm{O}\big(h^6\big), \tag{108}$$

$$\check{y}_{n+1} = 2y_n - y_{n-1} + \frac{h^2}{60}\Big[\widetilde{f}_{n+1} + 26 f_n + f_{n-1} + 16\big(\overline{f}_{n+1/2} + \overline{f}_{n-1/2}\big)\Big] + \mathrm{O}\big(h^8\big), \tag{109}$$

$$\widetilde{y}_{n+1/2} = \frac{1}{64}(19\check{y}_{n+1} + 58y_n - 13y_{n-1}) + \frac{h^2}{768}\big(-25\check{f}_{n+1} + 62 f_n + 23 f_{n-1}\big) + \mathrm{O}\big(h^8\big), \tag{110}$$

$$\widetilde{y}_{n-1/2} = \frac{1}{64}(-13\check{y}_{n+1} + 58y_n + 19y_{n-1}) + \frac{h^2}{768}\big(23\check{f}_{n+1} + 62 f_n - 25 f_{n-1}\big) + \mathrm{O}\big(h^8\big), \tag{111}$$

$$\overline{y}_{n+1/4} = \frac{1}{65536}(7405\check{y}_{n+1} + 67110y_n - 8979y_{n-1}) - \frac{h^2}{786432}\big(1289\check{f}_{n+1} - 27414 f_n - 1527 f_{n-1} + 24720\widetilde{f}_{n+1/2} - 31088\widetilde{f}_{n-1/2}\big) + \mathrm{O}\big(h^8\big), \tag{112}$$

$$\overline{y}_{n-1/4} = \frac{1}{65536}(-8979\check{y}_{n+1} + 67110y_n + 7405y_{n-1}) - \frac{h^2}{786432}\big(-1527\check{f}_{n+1} - 27414 f_n + 1289 f_{n-1} - 31088\widetilde{f}_{n+1/2} + 27420\widetilde{f}_{n-1/2}\big) + \mathrm{O}\big(h^8\big), \tag{113}$$

$$\widehat{y}_{n+1} = 2y_n - y_{n-1} + \frac{1}{3780}h^2\Big[47\big(\check{f}_{n+1} + f_{n-1}\big) + 3078 f_n + 1328\big(\widetilde{f}_{n+1/2} + \widetilde{f}_{n-1/2}\big) - 1024\big(\overline{f}_{n+1/4} + \overline{f}_{n-1/4}\big)\Big] + \mathrm{O}\big(h^{10}\big), \tag{114}$$

$$\check{y}_{n+1/2} = \frac{1}{2}\widehat{y}_{n+1} + \frac{1}{2}y_n + h^2\Big(-\frac{839}{120960}\hat{f}_{n+1} - \frac{333}{2240}f_n + \frac{17}{24192}f_{n-1} - \frac{4583}{30240}\widetilde{f}_{n+1/2} - \frac{593}{30240}\widetilde{f}_{n-1/2} + \frac{116}{945}\overline{f}_{n+1/4} + \frac{74}{945}\overline{f}_{n-1/4}\Big) + \mathrm{O}\big(h^{10}\big), \tag{115}$$

$$\check{y}_{n-1/2} = \frac{1}{2}y_n + \frac{1}{2}y_{n-1} + h^2\Big(\frac{17}{24192}\hat{f}_{n+1} - \frac{333}{2240}f_n - \frac{839}{120960}f_{n-1} - \frac{593}{30240}\widetilde{f}_{n+1/2} - \frac{4583}{30240}\widetilde{f}_{n-1/2} + \frac{74}{945}\overline{f}_{n+1/4} + \frac{116}{945}\overline{f}_{n-1/4}\Big) + \mathrm{O}\big(h^{10}\big), \tag{116}$$

$$\widetilde{y}_{n+1/4} = \frac{1}{4}\widehat{y}_{n+1} + \frac{3}{4}y_n + h^2\Big(-\frac{1979}{573440}\hat{f}_{n+1} - \frac{21993}{286720}f_n + \frac{1789}{5160960}f_{n-1} - \frac{101261}{1290240}\widetilde{f}_{n+1/2} - \frac{1389}{143360}\widetilde{f}_{n-1/2} + \frac{317}{8960}\overline{f}_{n+1/4} + \frac{3133}{80640}\overline{f}_{n-1/4}\Big) + \mathrm{O}\big(h^{10}\big), \tag{117}$$

$$\widetilde{y}_{n-1/4} = \frac{3}{4}y_n + \frac{1}{4}y_{n-1} + h^2\Big(\frac{1789}{5160960}\hat{f}_{n+1} - \frac{21993}{286720}f_n - \frac{1979}{573440}f_{n-1} - \frac{1389}{143360}\widetilde{f}_{n+1/2} - \frac{101261}{1290240}\widetilde{f}_{n-1/2} + \frac{3133}{80640}\overline{f}_{n+1/4} + \frac{317}{8960}\overline{f}_{n-1/4}\Big) + \mathrm{O}\big(h^{10}\big), \tag{118}$$

$$\overline{y}_{n+1/8} = \frac{1}{8}\widehat{y}_{n+1} + \frac{7}{8}y_n + h^2\Big(-\frac{981067}{566231040}\hat{f}_{n+1} - \frac{456099}{10485760}f_n + \frac{101237}{566231040}f_{n-1} - \frac{5507449}{141557760}\widetilde{f}_{n+1/2} - \frac{713689}{41557760}\widetilde{f}_{n-1/2} + \frac{122333}{8847360}\overline{f}_{n+1/4} + \frac{181229}{8847360}\overline{f}_{n-1/4}\Big) + \mathrm{O}\big(h^{10}\big), \tag{119}$$

$$\overline{y}_{n-1/8} = \frac{7}{8}y_n + \frac{1}{8}y_{n-1} + h^2\Big(\frac{101237}{566231040}\hat{f}_{n+1} - \frac{456099}{10485760}f_n - \frac{981067}{566231040}f_{n-1} - \frac{713689}{141557760}\widetilde{f}_{n+1/2} - \frac{5507449}{141557760}\widetilde{f}_{n-1/2}\frac{181229}{8847360}\overline{f}_{n+1/4} + \frac{122333}{8847360}\overline{f}_{n-1/4}\Big) + \mathrm{O}\big(h^{10}\big), \tag{120}$$

$$y_{n+1} - 2y_n + y_{n-1} = h^2\Big[\tfrac{623}{72900}\big(\hat{f}_{n+1} + f_{n-1}\big) - \tfrac{2675}{126} f_n + \tfrac{28828}{42525}\big(\check{f}_{n+1/2} + \check{f}_{n-1/2}\big) - \tfrac{233728}{42525}\big(\widetilde{f}_{n+1/4} + \widetilde{f}_{n-1/4}\big) + \tfrac{2031616}{127575}\big(\overline{f}_{n+1/8} + \overline{f}_{n-1/8}\big)\Big] + \mathrm{O}\big(h^{12}\big). \quad (121)$$

We observe that the above family of methods contains free parameters w_i.

The local truncation error of the new family of methods is given by

$$-\tfrac{1}{15018056692531200000}h^{12}\big[1683352125y^{(12)}(x) + 478271971485y^{(10)}(x) + 12815520402080y^{(8)}(x) + 595603836317952y^{(6)}(x) + 992673060529920y^{(4)}(x) + 1191207672635904 00w_i\, y^{(4)}(x)\big]. \quad (122)$$

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