Applied Mathematics and Computation 316 (2018) 296–309

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

How many k-step linear block methods exist and which of them is the most efficient and simplest one?

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ARTICLE INFO

Keywords:
Ordinary differential equations
Initial value problems
k-step block methods
Efficient formulation

ABSTRACT

There have appeared in the literature a lot of k-step block methods for solving initial-value problems. The methods consist in a set of k simultaneous multistep formulas over k non-overlapping intervals. A feature of block methods is that there is no need of other procedures to provide starting approximations, and thus the methods are self-starting (sharing this advantage of Runge–Kutta methods). All the formulas are usually obtained from a continuous approximation derived via interpolation and collocation at $k+1$ points. Nevertheless, all the k-step block methods thus obtained may be considered as different formulations of one of them, which results to be the most efficient and simple formulation of all of them. The theoretical analysis and the numerical experiments presented support this claim.

1. Introduction

Consider a first-order initial value problem (I.V.P.) of the form

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

on a given interval $[x_0, b] \in \mathbb{R},$ where conditions about the existence of a unique solution are assumed.

Among the numerical methods available in literature for solving the problem in (1) are the block methods. Block methods were proposed firstly by Milne [1]. They have the advantages of being more efficient in terms of cost implementation, time of execution and accuracy, and were developed to tackle some of the setbacks of predictor-corrector methods [2–7]. The block methods contain main and additional methods, a concept that is due to Brugnano and Trigiante [8]. They have appeared in literature dozens of block methods. This paper aims at analyzing and classifying these methods to show that most of them are the same. In fact, we will see that for each $k \in \mathbb{N}, k \geq 2,$ there is only one k-step method that is the simplest one.

The paper is organized as follows. In Section 2, we made a detailed analysis of 2-step block methods, showing that different methods appeared in literature in fact correspond to different formulations of the same method. Among these formulations there is only one which is the most efficient in terms of computational cost. In Section 3, the above analysis is extended to k-step block methods, obtaining a similar conclusion that there is only one of these methods which is the

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http://dx.doi.org/10.1016/j.amc.2017.08.036

most efficient. Some numerical examples are considered in Section 4 to show the performance of the different formulations of block methods. Finally, some conclusions are outlined in Section 5.

2. Analysis of the 2-step block methods

The first appearance of a 2-step block method seems to have been in [9] attributed to B. Dimsdale and R. F. Clippinger, where the method was written in the form

$$\begin{cases} y_{n+1} - \frac{1}{2} y_{n+2} = \frac{1}{2} y_n + \frac{h}{4} f_n - \frac{h}{4} f_{n+2} \\ y_{n+2} = y_n + \frac{h}{3}(f_n + 4f_{n+1} + f_{n+2}). \end{cases} \tag{2}$$

This method was mentioned also in [5], and later in [2], where the two previous works were cited.

Later, Onumanyi et al. in [10] presented the 2-block method given by the two formulas

$$\begin{cases} y_{n+1} = y_n + \frac{h}{12}(5f_n + 8f_{n+1} - f_{n+2}) \\ y_{n+2} = y_{n+1} + \frac{h}{12}(-f_n + 8f_{n+1} + 5f_{n+2}). \end{cases} \tag{3}$$

This 2-step block method has also appeared in [11–13] and [14].

Finally, in [15] Hongjiong and Bailin presented the 2-step block method that follows

$$\begin{cases} y_{n+1} = y_n + \frac{h}{12}(5f_n + 8f_{n+1} - f_{n+2}) \\ y_{n+2} = y_n + \frac{h}{3}(f_n + 4f_{n+1} + f_{n+2}). \end{cases} \tag{4}$$

Although we have made a vast searching, it possibly might have some other 2-step block methods of this kind in literature. What is the difference between these methods? Are there more possibilities? Which of them is the most efficient? To answer these questions we are going to proceed in developing all the 2-step block methods which are similar in appearance to the ones presented above.

We consider the grid points given by $x_n, x_{n+1} = x_n + h, x_{n+2} = x_n + 2h$. For solving the problem in (1) on the interval $[x_n, x_{n+2}]$ we consider the approximation of its solution $y(x)$ by a polynomial $p(x)$ given by

$$y(x) \simeq p(x) = \sum_{j=0}^{3} a_j x^j, \tag{5}$$

where the $a_j \in \mathbb{R}$, are real unknown parameters to be determined. The usual way to determine the values of these parameters relies on imposing appropriate collocation conditions to $p(x)$ and $p'(x)$ at the points x_n, x_{n+1}, x_{n+2}. Choosing four equations of the set

$$\left\{ p(x_n + ih) = y_{n+i}\, ,\, p'(x_n + ih) = f_{n+i} \right\}, \quad i = 0, 1, 2$$

where as usually y_{n+i} and f_{n+i} are approximations for the solution and the derivative at the given points, $y_{n+i} \simeq y(x_n + ih)$, $f_{n+i} \simeq y'(x_n + ih) = f(x_n + ih, y(x_n + ih))$, we obtain a system of four algebraic equations in four unknowns (the a_j , $j = 0, 1, 2, 3$). After solving the above system we substitute the obtained values in the polynomial $p(x)$, and the remaining two equations after substituting the a_j will constitute the block method. All of the 2-step block methods shown before may be obtained in this way.

The collocation conditions are given explicitly by

$$\begin{aligned} & a_0 + x_n a_1 + x_n^2 a_2 + x_n^3 a_3 - y_n = 0 \\ & a_0 + x_{n+1} a_1 + x_{n+1}^2 a_2 + x_{n+1}^3 a_3 - y_{n+1} = 0 \\ & a_0 + x_{n+2} a_1 + x_{n+2}^2 a_2 + x_{n+2}^3 a_3 - y_{n+2} = 0 \\ & a_1 + 2x_n a_2 + 3x_n^2 a_3 - f_n = 0 \\ & a_1 + 2x_{n+1} a_2 + 3x_{n+1}^2 a_3 - f_{n+1} = 0 \\ & a_1 + 2x_{n+2} a_2 + 3x_{n+2}^2 a_3 - f_{n+2} = 0. \end{aligned}$$

which may be written in matrix form as $\mathbf{A}_2\,\mathbf{y}_2=\mathbf{0}$, where

$$\mathbf{A}_2=\begin{pmatrix}1 & x_n & x_n^2 & x_n^3 & -1 & 0 & 0 & 0 & 0 & 0\\ 1 & x_{n+1} & x_{n+1}^2 & x_{n+1}^3 & 0 & -1 & 0 & 0 & 0 & 0\\ 1 & x_{n+2} & x_{n+2}^2 & x_{n+2}^3 & 0 & 0 & -1 & 0 & 0 & 0\\ 0 & 1 & 2x_n & 3x_n^2 & 0 & 0 & 0 & -1 & 0 & 0\\ 0 & 1 & 2x_{n+1} & 3x_{n+1}^2 & 0 & 0 & 0 & 0 & -1 & 0\\ 0 & 1 & 2x_{n+2} & 3x_{n+2}^2 & 0 & 0 & 0 & 0 & 0 & -1\end{pmatrix},$$

and $\mathbf{y}_2=(a_0,a_1,a_2,a_3,y_n,y_{n+1},y_{n+2},f_n,f_{n+1},f_{n+2})^T$.

It is obvious that the rank of the matrix $\mathbf{A}_2$ is six, and the system has a unique indeterminate solution. Thus, choosing any of the six columns as principal variables, we will obtain the solutions in terms of these variables. Four of these principal variables must be chosen to be the parameters a_j , $j=0,1,2,3$ in order to have the appropriate expression for the polynomial, and the other two solutions of the remaining principal variables give the two formulas that constituent the different 2-step block methods. In this way, the total of possibilities is $\binom{6}{2}=15$, which results in as many 2-step block methods, but in fact all of them are equivalent.

From all the 15 possible equivalent formulations of 2-step block methods, the simplest one will be that in which the number of evaluations of the function f is the lowest. There is only one possibility and corresponds to select as principal variables in the above system the a_j , $j=0,1,2,3$ and the f_{n+1},f_{n+2}. Thus the simplest formulation of the 2-step block methods is the following

$$\begin{cases}-5y_n+4y_{n+1}+y_{n+2}-2\,hf_n=4\,hf_{n+1}\\ 2y_n-4y_{n+1}+2y_{n+2}+hf_n=hf_{n+2}.\end{cases}\tag{6}$$

Note that in order to advance the solution in the block interval $[x_n,x_{n+2}]$ we have to solve the system in (6) for which a Newton-type method is usually appropriate. The y_n and f_n in (6) are constants, the y_{n+1} and y_{n+2} are the variables and thus the nonlinearity of the function f is reflected only two times in the system. On the contrary, in any other formulation of the 2-step block method the occurrences of the function f is higher, and may complicate the system, and thus its resolution.

3. Analysis of k-step block methods

For other than 2-step block methods the situation is similar, having a lot of different formulations. For example, in [13,15–21] there are different formulations of 3-step block methods, being the most common

$$\begin{cases}y_{n+1}=y_n+\dfrac{h}{24}\,(9f_n+19f_{n+1}-5f_{n+2}+f_{n+3})\\ y_{n+2}=y_n+\dfrac{h}{3}\,(f_n+4f_{n+1}+f_{n+2})\\ y_{n+3}=y_n+\dfrac{h}{8}\,(3f_n+9f_{n+1}+9f_{n+2}+3f_{n+3}).\end{cases}\tag{7}$$

Nevertheless, the simplest formulation of the above method is given by

$$\begin{cases}18\,hf_{n+1}=-6\,hf_n-17y_n+9y_{n+1}+9y_{n+2}-y_{n+3}\\ 9hf_{n+2}=3\,hf_n+7y_n-18y_{n+1}+9y_{n+2}+2y_{n+3}\\ 6hf_{n+3}=-6\,hf_n-13y_n+27y_{n+1}-27y_{n+2}+13y_{n+3}.\end{cases}\tag{8}$$

For the k-step block methods, $k\in\mathbb{N}$, we may follow a similar approach as before. We consider the grid points given by $x_n,x_{n+1}=x_n+h,\ldots,x_{n+k}=x_n+kh$. For solving the problem in (1) on the interval $[x_n,x_{n+k}]$ we consider the approximation of its solution $y(x)$ by a polynomial $p(x)$ given by

$$y(x)\simeq p(x)=\sum_{j=0}^{k+1}a_j\,x^j\,,\tag{9}$$

with the $a_j\in\mathbb{R}$ real unknown parameters to be determined. The usual way to determine the values of these parameters relies on imposing appropriate collocation conditions to $p(x)$ and $p'(x)$ at the points $x_n,x_{n+1},\ldots,x_{n+k}$. Choosing $k+2$ equations of the set

$$\left\{p(x_n+ih)=y_{n+i}\,,\,p'(x_n+ih)=f_{n+i}\right\},\quad i=0,1,\ldots,k$$

we get a system of $k+2$ algebraic equations in $k+2$ unknowns (the a_j , $j=0,1,\ldots,k$). After solving the above system we substitute the obtained values in the polynomial $p(x)$, and the remaining k equations (of the total set of $2k+2$) after substituting the a_j's, will constitute the block method. Any of the k-step block methods may be obtained in this way.

The collocation conditions are given by

$$\begin{aligned}
&a_0 + x_n a_1 + x_n^2 a_2 + x_n^3 a_3 + \cdots + x_n^{k+1} a_{k+1} - y_n = 0\\
&a_0 + x_{n+1} a_1 + x_{n+1}^2 a_2 + x_{n+1}^3 a_3 + \cdots + x_{n+1}^{k+1} a_{k+1} - y_{n+1} = 0\\
&\cdots\\
&a_0 + x_{n+k} a_1 + x_{n+k}^2 a_2 + x_{n+k}^3 a_3 + \cdots + x_{n+k}^{k+1} a_{k+1} - y_{n+k} = 0\\
&a_1 + 2x_n a_2 + 3x_n^2 a_3 + \cdots + (k+1) x_n^k a_{k+1} - f_n = 0\\
&a_1 + 2x_{n+1} a_2 + 3x_{n+1}^2 a_3 + \cdots + (k+1) x_{n+1}^k a_{k+1} - f_{n+1} = 0\\
&\cdots\\
&a_1 + 2x_{n+k} a_2 + 3x_{n+k}^2 a_3 + \cdots + (k+1) x_{n+k}^k a_{k+1} - f_{n+k} = 0.
\end{aligned}$$

which may be written in matrix form as $\mathbf{A}_k \, \mathbf{y}_k = \mathbf{0}$, where

$$\mathbf{A}_k = \begin{pmatrix}
1 & x_n & x_n^2 & \cdots & x_n^{k+1} & -1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0\\
1 & x_{n+1} & x_{n+1}^2 & \cdots & x_{n+1}^{k+1} & 0 & -1 & \cdots & 0 & 0 & 0 & \cdots & 0\\
\vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots\\
1 & x_{n+k} & x_{n+k}^2 & \cdots & x_{n+k}^{k+1} & 0 & 0 & \cdots & -1 & 0 & 0 & \cdots & 0\\
0 & 1 & 2x_n & \cdots & (k+1)x_n^k & 0 & 0 & \cdots & 0 & -1 & 0 & \cdots & 0\\
0 & 1 & 2x_{n+1} & \cdots & (k+1)x_{n+1}^k & 0 & 0 & \cdots & 0 & 0 & -1 & \cdots & 0\\
\vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots\\
0 & 1 & 2x_{n+k} & \cdots & (k+1)x_{n+k}^k & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & -1
\end{pmatrix},$$

and $\mathbf{y}_k = \left(a_0, a_1, a_2, \ldots, a_{k+1}, y_n, y_{n+1}, \ldots, y_{n+k}, f_n, f_{n+1}, \ldots, f_{n+k}\right)^T$.

It is obvious that the rank of the matrix $\mathbf{A}_k$ is $2k+2$, and the system has a unique indeterminate solution. Thus, choosing any of the $2k+2$ columns as principal variables, we will obtain the solutions in terms of these variables. From these principal variables $k+2$ must be chosen to be the parameters a_j , $j = 0, 1, \ldots, k+1$ in order to have the appropriate expression for the polynomial, and the other k solutions of the remaining principal variables give the k formulas that constituent the different k-step block methods. In this way, the total of possibilities is $\binom{2k+2}{k}$, which results in as many k-step block methods, but in fact all of them are equivalent.

From all the $\binom{2k+2}{k}$ possible equivalent formulations of k-step block methods, the simplest one will be that in which the number of evaluations of the function f is the lowest. There is only one possibility and corresponds to select as principal variables in the above system the a_j , $j = 0, 1, \ldots, k$ and the $f_{n+1}, \ldots, f_{n+k}$. In this way the nonlinearity of the function f is reflected only once in each of the equations of the block method.

Concerning the features of the k-step block methods, it can be shown that they are A-stable and of order $k+1$. Details on stability analysis can be found in the works by Akinfenwa et al. among others [22,23]. We will show how to proceed in the case for $k = 2$, but the procedure is the same for any k. For completeness we also have included in an appendix the simplest formulation of the block methods until $k = 10$, together with the local truncation errors and the stability functions.

Note that in its simplest form any k-step block method consists on a set of k linear formulas of the form

$$hf_{n+i} = F_i(y_n, y_{n+1}, \ldots, y_{n+k}, hf_n)\,, \quad i = 1, \ldots, k.$$

For each of the above formulas we consider a functional operator of the form

$$\mathcal{L}_i^k[z(x); h] = hz'(x+ih) - F_i\Big[z(x), z(x+h), \ldots, z(x+kh), hz'(x)\Big] \tag{10}$$

with $i = 1, 2, \ldots, k$, where $z(x)$ is an arbitrary analytic function defined on $[x_0, x_N]$, and F_i is the corresponding linear function on the right hand side of each formula with the approximate values replaced by the exact ones. Expanding the above expressions by Taylor's series around x and collecting terms in h, after substituting $z(x)$ by the true solution $y(x)$ of (1) and x by x_n we obtain the expressions for the local truncation errors, which may be arranged in vector form as

$$LTE^k = \left(C_1^k, C_2^k, \ldots, C_k^k\right)^T y^{(k+2)}(x_n) h^{k+2} + \mathcal{O}\left(h^{k+3}\right).$$

For $k = 2$ we have that

$$LTE^2 = \left(-\frac{1}{24}, \frac{1}{6}\right)^T y^{(4)}(x_n) h^4 + \mathcal{O}\left(h^5\right),$$

indicating that it is a third order method. In the appendix one can verify the order of the simplest block methods until $k = 10$, being the algebraic order of the k-step method, $k+1$.

The linear stability analysis of a given numerical method is usually examined by applying it to the well-known Dahlquist's test equation given by

$$y' = \lambda y, \quad \mathrm{Re}(\lambda) < 0. \tag{11}$$

The true solution of this problem is $y(x) = e^{\lambda x}$, which will be damped out as $x \to \infty$. It is expected that the application of a given numerical method to this problem has the same behavior as the true solution of the problem. For $k = 2$ we will determine the region in which the method in (6) reproduces the behavior of the true solutions for the test problem.

After applying the method in (6) to the test problem in (11) and setting $\bar{h} = \lambda h$ it results that it may be arranged in vector form as

$$A_2 \begin{pmatrix} y_{n+1} \\ y_{n+2} \end{pmatrix} = B_2 \begin{pmatrix} y_{n-1} \\ y_n \end{pmatrix}$$

where A_2 is the following matrix

$$A_2 = \begin{pmatrix} \bar{h} - 1 & -\dfrac{1}{4} \\ 4 & \bar{h} - 2 \end{pmatrix}$$

and the matrix B_2 is given by

$$B_2 = \begin{pmatrix} 0 & \dfrac{1}{4}(-2\bar{h} - 5) \\ 0 & \bar{h} + 2 \end{pmatrix}.$$

Thus, the method applied to the test problem may be written finally as

$$\begin{pmatrix} y_{n+1} \\ y_{n+2} \end{pmatrix} = M_2(\bar{h}) \begin{pmatrix} y_{n-1} \\ y_n \end{pmatrix}$$

where $M_2(\bar{h}) = A_2^{-1} B_2$ is the stability matrix.

The behavior of the numerical solution will depend on the eigenvalues of this matrix, and the stability properties of the method will be characterized by the spectral radius, $\rho[M_k(\bar{h})]$. The region of absolute stability, S, is defined as (see Hairer and Wanner [25])

$$S = \left\{ \bar{h} \in \mathbb{C} : |\rho[M_k(\bar{h})]| < 1 \right\}.$$

The method is said to be $\mathcal{A}$-stable if the left-half complex plane is included in the region of absolute stability, that is, if $\mathbb{C}^- \subseteq S$.

After some calculus, it can be obtained that the dominant eigenvalue consists in the rational function (known as stability function)

$$\rho[M_2(\bar{h})] = \frac{\bar{h}^2 + 3\bar{h} + 3}{\bar{h}^2 - 3\bar{h} + 3}$$

which has modulus less than one on the left-half complex plane, and thus, according to the above definition, the method is $\mathcal{A}$-stable. Fig. 1 shows the stability region of the presented method. The stability functions for the simplest k-step block methods up to $k = 10$ are given in the appendix, being the same plot of the stability region for all of them.

4. Some numerical experiments

To see the performance of the block methods we have used in the numerical experiments the two-step block method *BLOCK*2 in (2), the simplest two-step block method *BLOCK2SIMP* in (6), a 10-step block method *BLOCK*10 obtained taking as principal variables in the system in Section 3 the a_j, $j = 0, 1, \ldots, 10$ and the $y_{n+1}, \ldots, y_{n+10}$, and finally the simplest 10-step block method *BLOCK*10*SIMP* (obtained taking as principal variables in the system in Section 3 the a_j, $j = 0, 1, \ldots, 10$ and the $f_{n+1}, \ldots, f_{n+10}$).

4.1. Example 1

Consider the IVP given by

$$y' = \frac{y(2xy + 1)}{x\left(x^3 y^3 - 2xy - 1\right)}, \quad y(1) = 1, \quad x \in [1, 100]$$

whose exact solution is given in implicit form by

$$F(x, y) = \frac{1}{3x^3 y^3} + \frac{1}{x^2 y^2} + \log(y) - \frac{4}{3} = 0.$$

We have taken fixed stepsizes $h = 1/20, 1/40, 1/80$. Fig. 2 shows an efficiency plot of the absolute global errors in logarithmic scale versus CPU times. We see that the simplest formulations perform much better than the other ones.

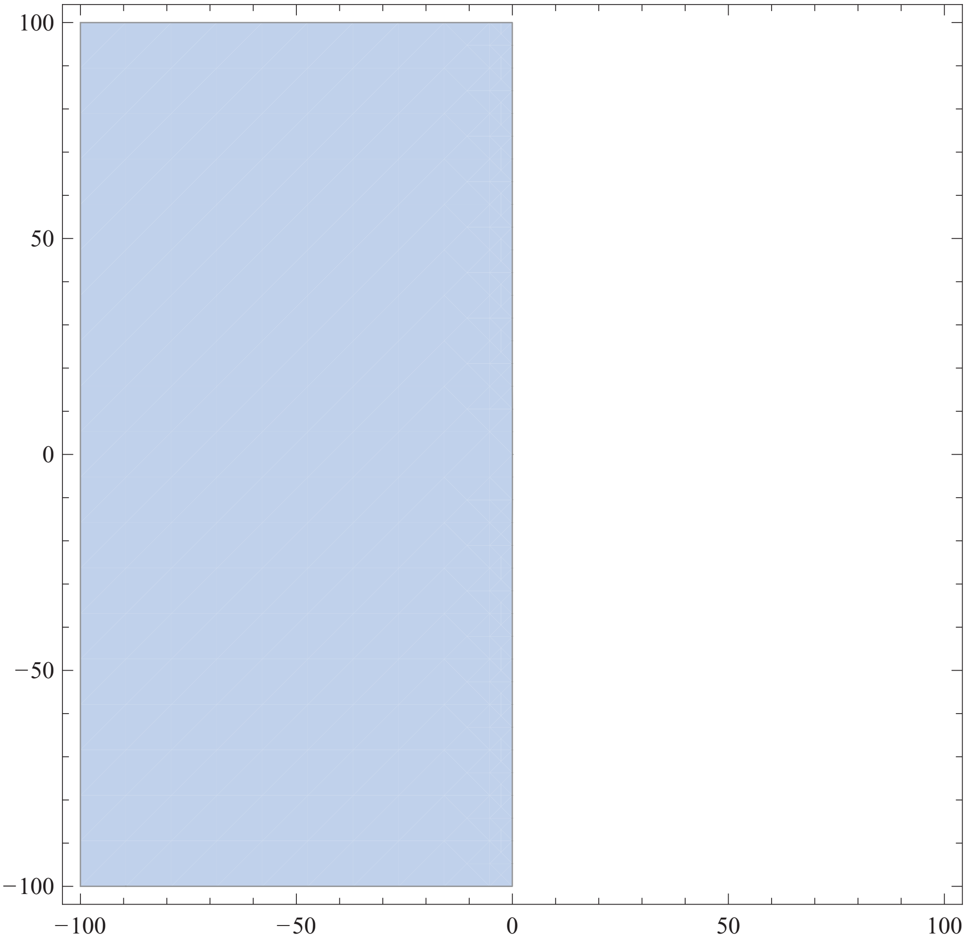

Fig. 1. Stability region of the proposed methods.

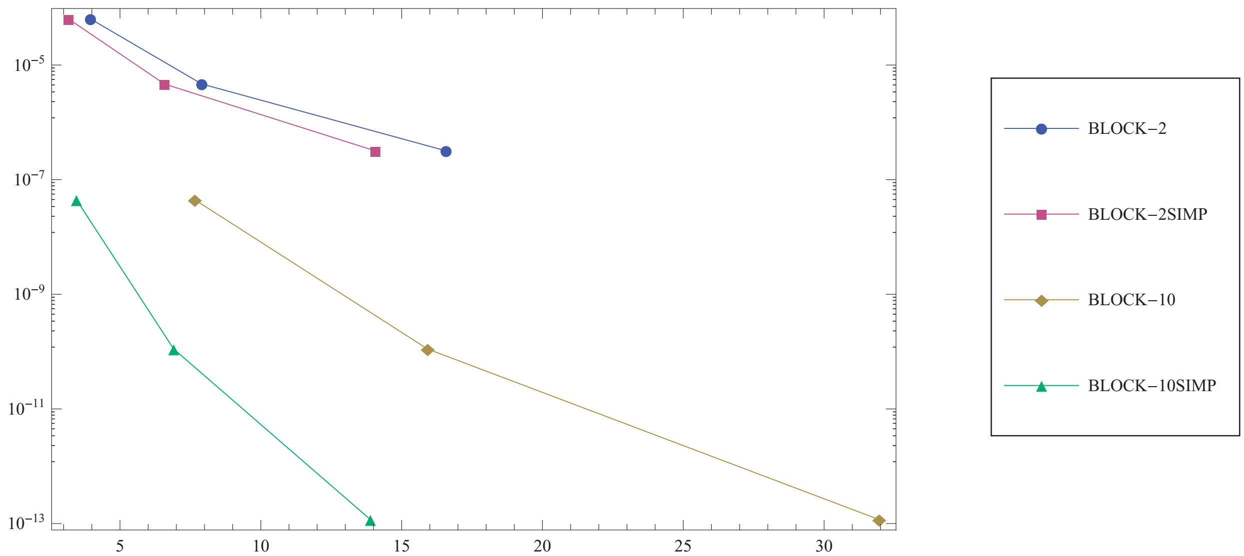

Fig. 2. Efficiency plot showing the absolute global error versus CPU time for Example 1.

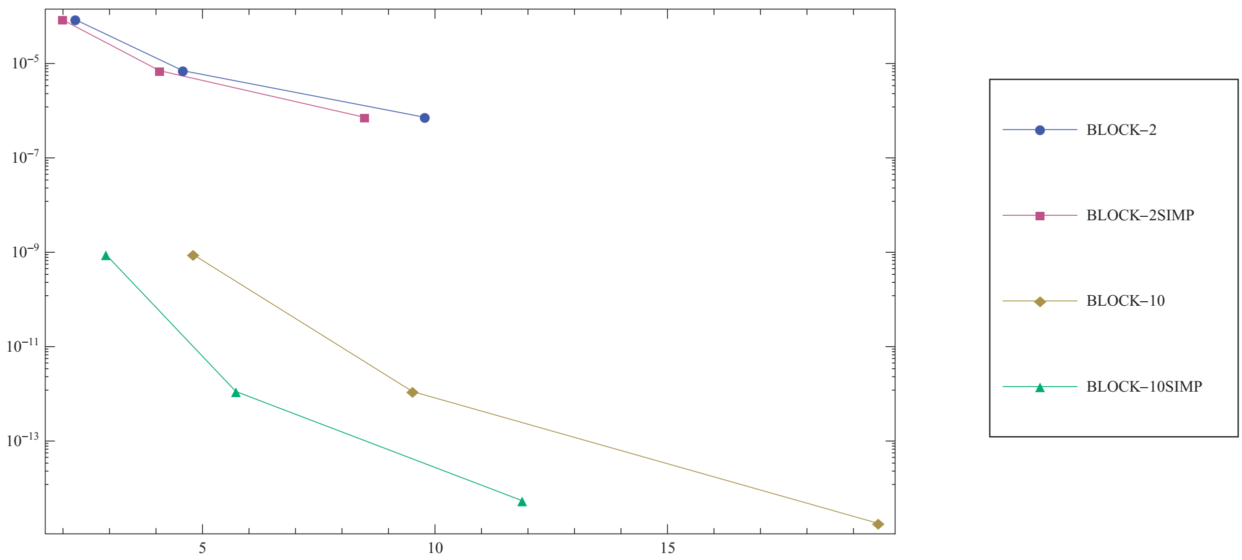

Fig. 3. Efficiency plot showing the absolute global error versus CPU time for Example 2.

4.2. Example

Now we have considered a system given by

$$\begin{aligned} y_1' &= -1002y_1 + 1000y_2^2, \quad y_1(0) = 1, \\ y_2' &= y_1 - y_2(1 + y_2), \quad y_2(0) = 1, \end{aligned}$$

whose exact solution is

$$\begin{aligned} y_1(x) &= e^{-2x}, \\ y_2(x) &= e^{-x}. \end{aligned}$$

The problem has been solved in the interval [0, 500] taking fixed stepsizes $h = 1/5, 1/10, 1/20$. We have considered the maximum norm in the errors, showing the efficiency plot of the errors in logarithmic scale versus CPU times in Fig. 3. We see that the performance has a similar behavior as in the previous example.

4.3. Example

The final example is a stiff parabolic equation with initial and boundary conditions, given by

$$\begin{aligned} &\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2}, \quad x \in [0, 1], t \in [0, 1] \\ &u(0, t) = u(1, t) = 0, \quad u(x, 0) = \sin(\pi x) + \sin(k\pi x), k \gg 1, \end{aligned}$$

whose exact solution is

$$u(x, t) = e^{-\pi^2 \nu t} \sin(\pi x) + e^{-k^2 \pi^2 \nu t} \sin(k\pi x).$$

For the numerical experiments we have taken $\nu = 1$ as in [24]. The procedure used to solve this problem consists in discretizing in space and then to apply the k-step block method, following a similar approach as in the method of lines. We take on the space domain a discrete mesh evenly spaced,

$$\Omega := \{x_0 \le x_1 \le \ldots \le x_{N+1} = b\},$$

in such a way that for every $x_i \in \Omega$, the second-order spatial derivative appearing in (12) is approximated by means of the finite difference

$$g''(x_i) = \frac{g(x_{i+1}) - 2g(x_i) + g(x_{i-1})}{(\triangle x)^2}.$$

Table 1
Maximum absolute errors at $t = 1$.

k	2-step block method	Best method in [24]
2	0.17×10^{-5}	0.74×10^{-5}
3	0.11×10^{-5}	0.74×10^{-5}
5	0.10×10^{-5}	0.74×10^{-5}
10	0.10×10^{-5}	0.74×10^{-5}

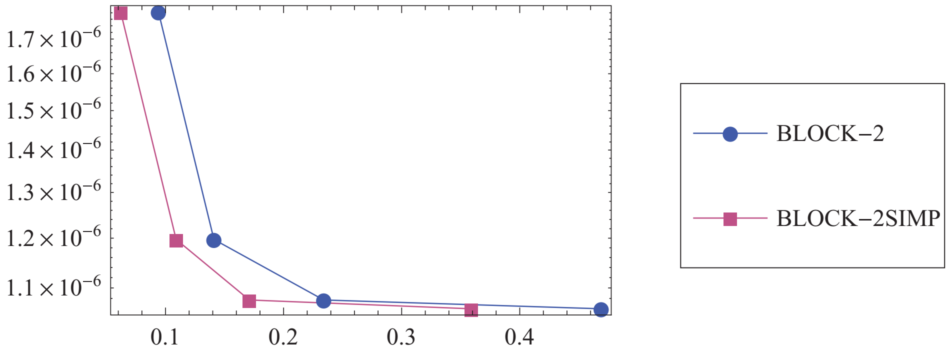

Fig. 4. Efficiency plot showing the absolute global error versus CPU time for Example 3.

Setting $u_i(t) = u(x_i, t)$ for $i = 1, \ldots, N$, with values $u_0(t) = u(0, t) = 0$, $u_{N+1}(t) = u(1, t) = 0$, having in mind the above discretization, the problem in (12) may be approximated by an initial-value problem of the form

$$\begin{cases} \dfrac{d\,\mathbf{u}}{d\,t} = A\,\mathbf{u}(t)\,, \\ \mathbf{u}(t_0) = (u_1(t_0), \ldots, u_N(t_0))^T\,, \end{cases} \tag{12}$$

where $\mathbf{u}(t) = (u_1(t), \ldots, u_N(t))^T$ and A is the tridiagonal matrix

$$A = \frac{1}{(\triangle x)^2}\begin{pmatrix} -2 & 1 & 0 & \ldots & 0 & 0 & 0 \\ 1 & -2 & 1 & \ldots & 0 & 0 & 0 \\ 0 & 1 & -2 & \ldots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & -2 & 1 & 0 \\ 0 & 0 & 0 & \ldots & 1 & -2 & 1 \\ 0 & 0 & 0 & \ldots & 0 & 1 & -2 \end{pmatrix}$$

where $\triangle x = 1/(N+1)$. We note that the eigenvalues of A are (see [26])

$$\lambda_i = \frac{-2}{(\triangle x)^2} + \frac{2}{(\triangle x)^2}\cos(i\pi\,\triangle x)\,, \qquad i = 1, \ldots, N\,,$$

which belong to the range $(-4\,(N+1)^2, 0)$, and so, for large values of N, the system becomes very stiff.

In the numerical experiments we have considered different values of k, and $\triangle x = 0.05$ as in [24], and $\triangle t = h = 1/(10k)$. In order to check the performance of the method a uniform step size has been used and the maximum absolute error has been computed at the final point $b = 1$ by

$$err = \max_{0 \le i \le N} |u_i(1) - u(x_i, 1)|\,, \tag{13}$$

where $u_i(1)$ is the numerical solution at time $t = 1$ and space x_i, and $u(x_i, 1)$ is the exact solution. The results with the methods for $k = 2$ in the previous sections are presented in Table 1 where we have included also the best results obtained in [24].

Fig. 4 shows the efficiency plot of the errors in logarithmic scale versus CPU times for the 2-step block methods in (3) and (6) considering the values of $k = 2, 3, 5, 10$ (from left to right). We see that the errors are the same, but the computational time needed by the simplest 2-step method is less, as expected.

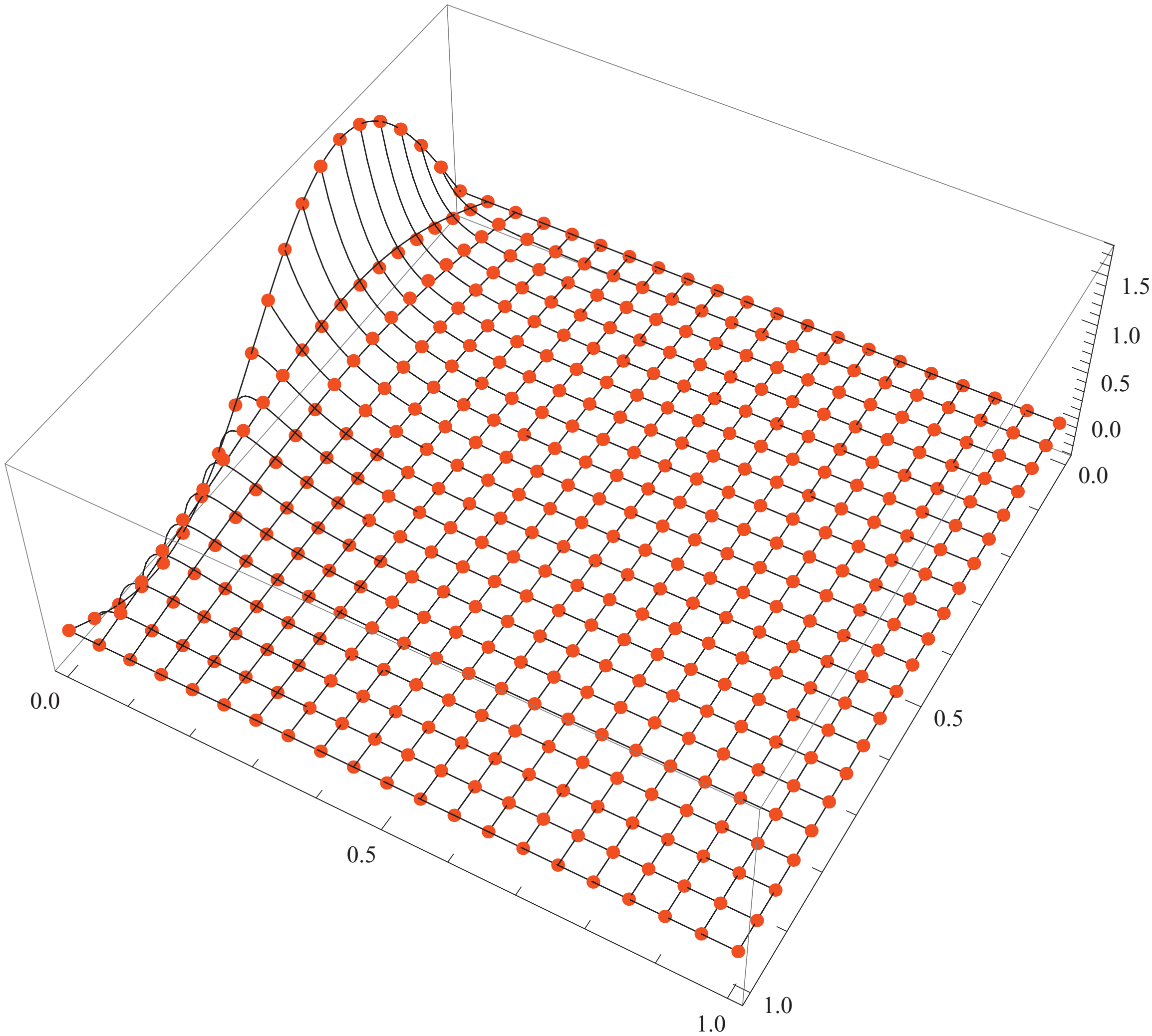

Fig. 5. Exact and discrete solutions for Example 3 with the 2-step block method taking $\triangle x = \triangle t = 0.05$.

Fig. 5 shows the exact graphical solution of the problem, and the numerical solution obtained on a uniform mesh with $\triangle x = \triangle t = 0.05$.

5. Conclusions

An analysis of k-step block methods has been done, showing that among all the possible formulations there is only one which is the most efficient, being all of them equivalent. To illustrate the performance of the methods considered, some numerical experiments have been presented. The numerical experiments support the claim that among the methods considered, the indicated ones are the most efficient.

Acknowledgments

The authors are grateful to one referee for several helpful suggestions that greatly improved the manuscript.

Appendix A. Simplest *k*-step block formulas, their truncation errors and stability functions.

k = 2:

$$4\ hf_{n+1} = -5y_n + 4y_{n+1} + y_{n+2} - 2\ hf_n$$

$$hf_{n+2} = 2y_n - 4y_{n+1} + 2y_{n+2} + hf_n.$$

$$LTE^2 = \left(-\frac{1}{24}, \frac{1}{6}\right)^T y^{(4)}(x_n)h^4 + \mathcal{O}\left(h^5\right),$$

$$\rho[M_2(\bar{h})] = \frac{\bar{h}^2 + 3\bar{h} + 3}{\bar{h}^2 - 3\bar{h} + 3}.$$

k = 3:

$$\begin{aligned}
18f_{n+1}h &= -17y_n + 9y_{n+1} + 9y_{n+2} - y_{n+3} - 6f_nh \\
9f_{n+2}h &= 3f_nh + 7y_n - 18y_{n+1} + 9y_{n+2} + 2y_{n+3} \\
6f_{n+3}h &= -6f_nh - 13y_n + 27y_{n+1} - 27y_{n+2} + 13y_{n+3}.
\end{aligned}$$

$$LTE^3 = \left(\frac{3}{10}, -\frac{3}{10}, \frac{9}{10}\right)^T y^{(5)}(x_n)h^5 + \mathcal{O}\left(h^6\right),$$

$$\rho[M_3(\bar{h})] = \frac{3\bar{h}^3 + 11\bar{h}^2 + 18\bar{h} + 12}{-3\bar{h}^3 + 11\bar{h}^2 - 18\bar{h} + 12}.$$

k = 4:

$$\begin{aligned}
48f_{n+1}h &= -12f_nh - 37y_n + 8y_{n+1} + 36y_{n+2} - 8y_{n+3} + y_{n+4} \\
72f_{n+2}h &= 12f_nh + 31y_n - 96y_{n+1} + 36y_{n+2} + 32y_{n+3} - 3y_{n+4} \\
48f_{n+3}h &= -12f_nh - 29y_n + 72y_{n+1} - 108y_{n+2} + 56y_{n+3} + 9y_{n+4} \\
3f_{n+4}h &= 3f_nh + 7y_n - 16y_{n+1} + 18y_{n+2} - 16y_{n+3} + 7y_{n+4}.
\end{aligned}$$

$$LTE^4 = \left(-\frac{2}{5}, \frac{4}{5}, -\frac{6}{5}, \frac{2}{5}\right)^T y^{(6)}(x_n)h^6 + \mathcal{O}\left(h^7\right),$$

$$\rho[M_4(\bar{h})] = \frac{12\bar{h}^4 + 50\bar{h}^3 + 105\bar{h}^2 + 120\bar{h} + 60}{12\bar{h}^4 - 50\bar{h}^3 + 105\bar{h}^2 - 120\bar{h} + 60}.$$

k = 5:

$$\begin{aligned}
300f_{n+1}h &= -60f_nh - 197y_n - 25y_{n+1} + 300y_{n+2} - 100y_{n+3} + 25y_{n+4} - 3y_{n+5} \\
600f_{n+2}h &= 60f_nh + 167y_n - 600y_{n+1} + 100y_{n+2} + 400y_{n+3} - 75y_{n+4} + 8y_{n+5} \\
600f_{n+3}h &= -60f_nh - 157y_n + 450y_{n+1} - 900y_{n+2} + 400y_{n+3} + 225y_{n+4} - 18y_{n+5} \\
75f_{n+4}h &= 15f_nh + 38y_n - 100y_{n+1} + 150y_{n+2} - 200y_{n+3} + 100y_{n+4} + 12y_{n+5} \\
60f_{n+5}h &= -60f_nh - 149y_n + 375y_{n+1} - 500y_{n+2} + 500y_{n+3} - 375y_{n+4} + 149y_{n+5}.
\end{aligned}$$

$$LTE^5 = \left(\frac{10}{7}, -\frac{20}{7}, \frac{30}{7}, -\frac{10}{7}, \frac{50}{7}\right)^T y^{(7)}(x_n)h^7 + \mathcal{O}\left(h^8\right),$$

$$\rho[M_5(\bar{h})] = \frac{60\bar{h}^5 + 274\bar{h}^4 + 675\bar{h}^3 + 1020\bar{h}^2 + 900\bar{h} + 360}{-60\bar{h}^5 + 274\bar{h}^4 - 675\bar{h}^3 + 1020\bar{h}^2 - 900\bar{h} + 360}.$$

$k = 6$:

$$\begin{aligned}
360f_{n+1}h &= -60f_nh - 207y_n - 102y_{n+1} + 450y_{n+2} - 200y_{n+3} + 75y_{n+4} - 18y_{n+5} + 2y_{n+6} \\
900f_{n+2}h &= 60f_nh + 177y_n - 720y_{n+1} - 75y_{n+2} + 800y_{n+3} - 225y_{n+4} + 48y_{n+5} - 5y_{n+6} \\
1200f_{n+3}h &= -60f_nh - 167y_n + 540y_{n+1} - 1350y_{n+2} + 400y_{n+3} + 675y_{n+4} - 108y_{n+5} + 10y_{n+6} \\
450f_{n+4}h &= 30f_nh + 81y_n - 240y_{n+1} + 450y_{n+2} - 800y_{n+3} + 375y_{n+4} + 144y_{n+5} - 10y_{n+6} \\
360f_{n+5}h &= -60f_nh - 159y_n + 450y_{n+1} - 750y_{n+2} + 1000y_{n+3} - 1125y_{n+4} + 534y_{n+5} + 50y_{n+6} \\
60f_{n+6}h &= 60f_nh + 157y_n - 432y_{n+1} + 675y_{n+2} - 800y_{n+3} + 675y_{n+4} - 432y_{n+5} + 157y_{n+6}.
\end{aligned}$$

$$LTE^6 = \left(-\frac{15}{14}, \frac{15}{7}, -\frac{45}{14}, \frac{15}{7}, -\frac{75}{14}, \frac{45}{7}\right)^T y^{(8)}(x_n)h^8 + \mathcal{O}\left(h^9\right),$$

$$\rho[M_6(\bar{h})] = \frac{30\bar{h}^6 + 147\bar{h}^5 + 406\bar{h}^4 + 735\bar{h}^3 + 875\bar{h}^2 + 630\bar{h} + 210}{30\bar{h}^6 - 147\bar{h}^5 + 406\bar{h}^4 - 735\bar{h}^3 + 875\bar{h}^2 - 630\bar{h} + 210}.$$

$k = 7$:

$$\begin{aligned}
2940f_{n+1}h &= -420f_nh - 1509y_n - 1323y_{n+1} + 4410y_{n+2} - 2450y_{n+3} + 1225y_{n+4} \\
&\quad -441y_{n+5} + 98y_{n+6} - 10y_{n+7} \\
8820f_{n+2}h &= 420f_nh + 1299y_n - 5880y_{n+1} - 2499y_{n+2} + 9800y_{n+3} - 3675y_{n+4} \\
&\quad +1176y_{n+5} - 245y_{n+6} + 24y_{n+7} \\
14700f_{n+3}h &= -420f_nh - 1229y_n + 4410y_{n+1} - 13230y_{n+2} + 1225y_{n+3} + 11025y_{n+4} \\
&\quad -2646y_{n+5} + 490y_{n+6} - 45y_{n+7} \\
7350f_{n+4}h &= 210f_nh + 597y_n - 1960y_{n+1} + 4410y_{n+2} - 9800y_{n+3} + 3675y_{n+4} \\
&\quad +3528y_{n+5} - 490y_{n+6} + 40y_{n+7} \\
8820f_{n+5}h &= -420f_nh - 1173y_n + 3675y_{n+1} - 7350y_{n+2} + 12250y_{n+3} - 18375y_{n+4} \\
&\quad +8673y_{n+5} + 2450y_{n+6} - 150y_{n+7} \\
2940f_{n+6}h &= 420f_nh + 1159y_n - 3528y_{n+1} + 6615y_{n+2} - 9800y_{n+3} + 11025y_{n+4} \\
&\quad -10584y_{n+5} + 4753y_{n+6} + 360y_{n+7} \\
420f_{n+7}h &= -420f_nh - 1149y_n + 3430y_{n+1} - 6174y_{n+2} + 8575y_{n+3} - 8575y_{n+4} \\
&\quad +6174y_{n+5} - 3430y_{n+6} + 1149y_{n+7}.
\end{aligned}$$

$$LTE^7 = \left(\frac{35}{6}, -\frac{35}{3}, \frac{35}{2}, -\frac{35}{3}, \frac{175}{6}, -35, \frac{245}{6}\right)^T y^{(9)}(x_n)h^9 + \mathcal{O}\left(h^{10}\right),$$

$$\rho[M_7(\bar{h})] = \frac{210\bar{h}^7 + 1089\bar{h}^6 + 3283\bar{h}^5 + 6769\bar{h}^4 + 9800\bar{h}^3 + 9660\bar{h}^2 + 5880\bar{h} + 1680}{-210\bar{h}^7 + 1089\bar{h}^6 - 3283\bar{h}^5 + 6769\bar{h}^4 - 9800\bar{h}^3 + 9660\bar{h}^2 - 5880\bar{h} + 1680}.$$

$k = 8$:

$$\begin{aligned}
6720f_{n+1}h &= -840f_nh - 3123y_n - 3984y_{n+1} + 11760y_{n+2} - 7840y_{n+3} + 4900y_{n+4} \\
&\quad -2352y_{n+5} + 784y_{n+6} - 160y_{n+7} + 15y_{n+8} \\
23520f_{n+2}h &= 840f_nh + 2703y_n - 13440y_{n+1} - 10584y_{n+2} + 31360y_{n+3} - 14700y_{n+4} \\
&\quad +6272y_{n+5} - 1960y_{n+6} + 384y_{n+7} - 35y_{n+8}
\end{aligned}$$

$$
\begin{aligned}
47040 f_{n+3} h &= -840 f_n h - 2563 y_n + 10080 y_{n+1} - 35280 y_{n+2} - 5488 y_{n+3} + 44100 y_{n+4} \\
&\quad -14112 y_{n+5} + 3920 y_{n+6} - 720 y_{n+7} + 63 y_{n+8} \\
58800 f_{n+4} h &= 840 f_n h + 2493 y_n - 8960 y_{n+1} + 23520 y_{n+2} - 62720 y_{n+3} + 14700 y_{n+4} \\
&\quad +37632 y_{n+5} - 7840 y_{n+6} + 1280 y_{n+7} - 105 y_{n+8} \\
47040 f_{n+5} h &= -840 f_n h - 2451 y_n + 8400 y_{n+1} - 19600 y_{n+2} + 39200 y_{n+3} - 73500 y_{n+4} \\
&\quad +30576 y_{n+5} + 19600 y_{n+6} - 2400 y_{n+7} + 175 y_{n+8} \\
23520 f_{n+6} h &= 840 f_n h + 2423 y_n - 8064 y_{n+1} + 17640 y_{n+2} - 31360 y_{n+3} + 44100 y_{n+4} \\
&\quad -56448 y_{n+5} + 26264 y_{n+6} + 5760 y_{n+7} - 315 y_{n+8} \\
6720 f_{n+7} h &= -840 f_n h - 2403 y_n + 7840 y_{n+1} - 16464 y_{n+2} + 27440 y_{n+3} - 34300 y_{n+4} \\
&\quad +32928 y_{n+5} - 27440 y_{n+6} + 11664 y_{n+7} + 735 y_{n+8} \\
210 f_{n+8} h &= 210 f_n h + 597 y_n - 1920 y_{n+1} + 3920 y_{n+2} - 6272 y_{n+3} + 7350 y_{n+4} \\
&\quad -6272 y_{n+5} + 3920 y_{n+6} - 1920 y_{n+7} + 597 y_{n+8}.
\end{aligned}
$$

$$
LTE^8 = \left(-\frac{28}{3}, \frac{56}{3}, -28, \frac{112}{3}, -\frac{140}{3}, 56, -\frac{196}{3}, \frac{56}{3}\right)^T y^{(10)}(x_n) h^{10} + \mathcal{O}\left(h^{11}\right),
$$

$$
\rho[M_8(\bar{h})] = \frac{P_8(\bar{h})}{Q_8(\bar{h})}, \text{ where}
$$

$$
\begin{aligned}
P_8(\bar{h}) &= 1680\bar{h}^8 + 9132\bar{h}^7 + 29531\bar{h}^6 + 67284\bar{h}^5 + 112245\bar{h}^4 + 136080\bar{h}^3 \\
&\quad +114660\bar{h}^2 + 60480\bar{h} + 15120, \\
Q_8(\bar{h}) &= 1680\bar{h}^8 - 9132\bar{h}^7 + 29531\bar{h}^6 - 67284\bar{h}^5 + 112245\bar{h}^4 - 136080\bar{h}^3 \\
&\quad +114660\bar{h}^2 - 60480\bar{h} + 15120.
\end{aligned}
$$

$k = 9$:

$$
\begin{aligned}
22680 f_{n+1} h &= -2520 f_n h - 9649 y_n - 16281 y_{n+1} + 45360 y_{n+2} - 35280 y_{n+3} + 26460 y_{n+4} \\
&\quad -15876 y_{n+5} + 7056 y_{n+6} - 2160 y_{n+7} + 405 y_{n+8} - 35 y_{n+9} \\
90720 f_{n+2} h &= 2520 f_n h + 8389 y_n - 45360 y_{n+1} - 53784 y_{n+2} + 141120 y_{n+3} - 79380 y_{n+4} \\
&\quad +42336 y_{n+5} - 17640 y_{n+6} + 5184 y_{n+7} - 945 y_{n+8} + 80 y_{n+9} \\
211680 f_{n+3} h &= -2520 f_n h - 7969 y_n + 34020 y_{n+1} - 136080 y_{n+2} - 59976 y_{n+3} + 238140 y_{n+4} \\
&\quad -95256 y_{n+5} + 35280 y_{n+6} - 9720 y_{n+7} + 1701 y_{n+8} - 140 y_{n+9} \\
317520 f_{n+4} h &= 2520 f_n h + 7759 y_n - 30240 y_{n+1} + 90720 y_{n+2} - 282240 y_{n+3} + 15876 y_{n+4} \\
&\quad +254016 y_{n+5} - 70560 y_{n+6} + 17280 y_{n+7} - 2835 y_{n+8} + 224 y_{n+9} \\
317520 f_{n+5} h &= -2520 f_n h - 7633 y_n + 28350 y_{n+1} - 75600 y_{n+2} + 176400 y_{n+3} - 396900 y_{n+4} \\
&\quad +127008 y_{n+5} + 176400 y_{n+6} - 32400 y_{n+7} + 4725 y_{n+8} - 350 y_{n+9} \\
211680 f_{n+6} h &= 2520 f_n h + 7549 y_n - 27216 y_{n+1} + 68040 y_{n+2} - 141120 y_{n+3} + 238140 y_{n+4} \\
&\quad -381024 y_{n+5} + 165816 y_{n+6} + 77760 y_{n+7} - 8505 y_{n+8} + 560 y_{n+9} \\
90720 f_{n+7} h &= -2520 f_n h - 7489 y_n + 26460 y_{n+1} - 63504 y_{n+2} + 123480 y_{n+3} - 185220 y_{n+4} \\
&\quad +222264 y_{n+5} - 246960 y_{n+6} + 112104 y_{n+7} + 19845 y_{n+8} - 980 y_{n+9} \\
5670 f_{n+8} h &= 630 f_n h + 1861 y_n - 6480 y_{n+1} + 15120 y_{n+2} - 28224 y_{n+3} + 39690 y_{n+4} \\
&\quad -42336 y_{n+5} + 35280 y_{n+6} - 25920 y_{n+7} + 10449 y_{n+8} + 560 y_{n+9} \\
2520 f_{n+9} h &= -2520 f_n h - 7409 y_n + 25515 y_{n+1} - 58320 y_{n+2} + 105840 y_{n+3} - 142884 y_{n+4} \\
&\quad +142884 y_{n+5} - 105840 y_{n+6} + 58320 y_{n+7} - 25515 y_{n+8} + 7409 y_{n+9}.
\end{aligned}
$$

$$LTE^9 = \left(\frac{252}{11}, -\frac{504}{11}, \frac{756}{11}, -\frac{1008}{11}, \frac{1260}{11}, -\frac{1512}{11}, \frac{1764}{11}, -\frac{504}{11}, \frac{2268}{11}\right)^T y^{(11)}(x_n)h^{11} + \mathcal{O}\left(h^{12}\right),$$

$$\rho[M_9(\bar{h})] = \frac{P_9(\bar{h})}{Q_9(\bar{h})}, \text{ where}$$

$$\begin{aligned} P_9(\bar{h}) &= 15120\bar{h}^9 + 85548\bar{h}^8 + 293175\bar{h}^7 + 723680\bar{h}^6 + 1346625\bar{h}^5 \\ &\quad + 1898190\bar{h}^4 + 1984500\bar{h}^3 + 1461600\bar{h}^2 + 680400\bar{h} + 151200, \\ Q_9(\bar{h}) &= -15120\bar{h}^9 + 85548\bar{h}^8 - 293175\bar{h}^7 + 723680\bar{h}^6 - 1346625\bar{h}^5 \\ &\quad + 1898190\bar{h}^4 - 1984500\bar{h}^3 + 1461600\bar{h}^2 - 680400\bar{h} + 151200. \end{aligned}$$

k = 10:

$$\begin{aligned}
-25200\ hf_{n+1} &= 2520\ hf_n + 9901y_n + 20890y_{n+1} - 28y_{n+10} - 56700y_{n+2} + 50400y_{n+3} \\ &\quad - 44100y_{n+4} + 31752y_{n+5} - 17640y_{n+6} + 7200y_{n+7} - 2025y_{n+8} + 350y_{n+9} \\
113400\ hf_{n+2} &= 2520\ hf_n + 8641y_n - 50400y_{n+1} - 63y_{n+10} - 81405y_{n+2} + 201600y_{n+3} \\ &\quad - 132300y_{n+4} + 84672y_{n+5} - 44100y_{n+6} + 17280y_{n+7} - 4725y_{n+8} + 800y_{n+9} \\
-302400\ hf_{n+3} &= 2520\ hf_n + 8221y_n - 37800y_{n+1} - 108y_{n+10} + 170100y_{n+2} + 128880y_{n+3} \\ &\quad - 396900y_{n+4} + 190512y_{n+5} - 88200y_{n+6} + 32400y_{n+7} - 8505y_{n+8} + 1400y_{n+9} \\
529200\ hf_{n+4} &= 2520\ hf_n + 8011y_n - 33600y_{n+1} - 168y_{n+10} + 113400y_{n+2} - 403200y_{n+3} \\ &\quad - 61740y_{n+4} + 508032y_{n+5} - 176400y_{n+6} + 57600y_{n+7} - 14175y_{n+8} + 2240y_{n+9} \\
635040\ hf_{n+5} &= -2520\ hf_n - 7885y_n + 31500y_{n+1} + 252y_{n+10} - 94500y_{n+2} + 252000y_{n+3} \\ &\quad - 661500y_{n+4} + 127008y_{n+5} + 441000y_{n+6} - 108000y_{n+7} + 23625y_{n+8} - 3500y_{n+9} \\
529200\ hf_{n+6} &= 2520hf_n + 7801y_n - 30240y_{n+1} - 378y_{n+10} + 85050y_{n+2} - 201600y_{n+3} \\ &\quad + 396900y_{n+4} - 762048y_{n+5} + 282240y_{n+6} + 259200y_{n+7} - 42525y_{n+8} + 5600y_{n+9} \\
302400\ hf_{n+7} &= -2520\ hf_n - 7741y_n + 29400y_{n+1} + 588y_{n+10} - 79380y_{n+2} + 176400y_{n+3} \\ &\quad - 308700y_{n+4} + 444528y_{n+5} - 617400y_{n+6} + 272880y_{n+7} + 99225y_{n+8} - 9800y_{n+9} \\
14175\ hf_{n+8} &= 315\ hf_n + 962y_n - 3600y_{n+1} - 126y_{n+10} + 9450y_{n+2} - 20160y_{n+3} \\ &\quad + 33075y_{n+4} - 42336y_{n+5} + 44100y_{n+6} - 43200y_{n+7} + 19035y_{n+8} + 2800y_{n+9} \\
25200\ hf_{n+9} &= -2520\ hf_n - 7661y_n + 28350y_{n+1} + 2268y_{n+10} - 72900y_{n+2} + 151200y_{n+3} \\ &\quad - 238140y_{n+4} + 285768y_{n+5} - 264600y_{n+6} + 194400y_{n+7} - 127575y_{n+8} + 48890y_{n+9} \\
2520\ hf_{n+10} &= 2520\ hf_n + 7633y_n - 28000y_{n+1} + 7633y_{n+10} + 70875y_{n+2} - 144000y_{n+3} \\ &\quad + 220500y_{n+4} - 254016y_{n+5} + 220500y_{n+6} - 144000y_{n+7} + 70875y_{n+8} - 28000y_{n+9}
\end{aligned}$$

$$LTE^{10} = \left(\frac{-210}{11}, \frac{420}{11}, \frac{-630}{11}, \frac{840}{11}, \frac{-1050}{11}, \frac{1260}{11}, \frac{-1470}{11}, \frac{210}{11}, \frac{-1890}{11}, \frac{2100}{11}\right)^T y^{(12)}(x_n)h^{12} + \mathcal{O}\left(h^{13}\right),$$

$$\rho[M_{10}(\bar{h})] = \frac{P_{10}(\bar{h})}{Q_{10}(\bar{h})}, \text{ where}$$

$$\begin{aligned} P_{10}(\bar{h}) &= 75600\bar{h}^{10} + 442860\bar{h}^9 + 1594197\bar{h}^8 + 4204750\bar{h}^7 + 8542325\bar{h}^6 + 13530825\bar{h}^5 \\ &\quad + 16566165\bar{h}^4 + 15246000\bar{h}^3 + 9979200\bar{h}^2 + 4158000\bar{h} + 831600, \\ Q_{10}(\bar{h}) &= 75600\bar{h}^{10} - 442860\bar{h}^9 + 1594197\bar{h}^8 - 4204750\bar{h}^7 + 8542325\bar{h}^6 - 13530825\bar{h}^5 \\ &\quad + 16566165\bar{h}^4 - 15246000\bar{h}^3 + 9979200\bar{h}^2 - 4158000\bar{h} + 831600. \end{aligned}$$

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